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

SUPPORTING INFORMATION

Evaluation of Packing Single and Multiple Atoms and Molecule in the Porous Organic Cage **CC3**-*R*

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Table S1. More complete Table 1 with Point Groups, Relative Energies (kcal/mol), Enthalpies (kcal/mol), and Free Energies (kcal/mol) with Respect to **CC3**-*R* and Varies Encapsulated Species per Unit[a]

	PG	M06-2X/ 6-31G(d)	B3LYP/6-31G(d,p)-D3BJ//M06-2X/6-31G(d)						
		ΔE	BSSE/2	ΔE+ BSSE/2	ΔH (298K)	ΔG (100K)	ΔG (200K)	ΔG (300K)	ΔG (400K)
CH_4	T_d								
$HCCl_3$	C_{3v}								
Xe	K								
Kr	K								
CO_2	D_{ih}								
C_2H_2	D_{ih}								
H_2O									
SF_6	O_h								
5-^{t}Bu-*m*-xylene	C_s								
CC3-R	T								
Xe@**CC3**	T	-7.73	2.39	-10.66	-10.33	-8.56	-6.79	-5.02	-3.24
3Xe@**CC3**	C_3	-6.44	2.04	-7.68	-7.41	-5.25	-3.09	-0.92	1.24
4Xe@**CC3**	T	-6.64	1.53	-8.17	-8.42	-6.27	-4.13	-1.98	0.17
4Xe@**CC3**	C_1	-6.66	1.53	-8.17	-7.88	-5.67	-3.45	-1.24	0.97
5Xe@**CC3**	T	-5.85	1.50	-7.66	-7.69	-5.31	-2.93	-0.55	1.82
5Xe@**CC3**	C_1	-5.88	1.49	-7.65	-7.27	-5.06	-2.84	-0.63	1.59
Kr@**CC3**	T	-4.40	1.24	-6.75	-6.42	-4.15	-1.88	0.39	2.67
4Kr@**CC3**	T	-4.45	0.94	-6.04	-5.81	-3.62	-1.43	0.76	2.95
5Kr@**CC3**	T	-3.85	0.89	-5.56	-5.25	-3.15	-1.04	1.07	3.17
SF_6@**CC3**-TS	C_3	-4.04	2.38	-6.49	-7.10	-4.35	-1.60	1.15	3.91
SF_6@**CC3**-TS	C_1	-6.07	3.53	-7.91	-7.08	-4.16	-1.24	1.69	4.61
SF_6@**CC3**	T	-9.74	4.53	-15.32	-14.25	-11.90	-9.56	-7.21	-4.86
4SF_6@**CC3**	T	-9.31	4.97	-10.80	-9.47	-5.82	-2.18	1.47	5.12
5SF_6@**CC3**	T	-10.07	4.31	-13.64	-12.72	-9.57	-6.41	-3.26	-0.10
5SF_6@**CC3**	C_3	-10.25	4.31	-13.27	-11.92	-8.52	-5.12	-1.73	1.67
$(SF_6)_4^h$	T	-0.93	0.57	-1.18	-0.33	0.71	1.75	2.79	5.02
$(SF_6)_5^h$	D_2	-1.96	1.30	-1.47	-0.67	0.97	2.61	4.25	5.89
$(SF_6)_5^h$	C_2	-1.99	1.30	-1.47	-0.54	1.29	3.12	4.96	6.79
CH_4@**CC3**	T	-3.02	0.73	-5.24	-5.79	-4.33	-2.86	-1.40	0.07
CH_4@**CC3**	C_3	-4.40	1.02	-5.52	-4.24	-2.58	-0.91	0.75	2.42
3CH_4@**CC3**	C_3	-4.66	0.99	-5.99	-4.85	-2.64	-0.42	1.80	4.01
4CH_4@**CC3**-a	T	-4.57	1.01	-6.02	-5.74	-3.62	-1.50	0.62	2.74
4CH_4@**CC3**-b	T	-4.67	0.98	-5.96	-4.78	-2.39	-0.01	2.38	4.76
5CH_4@**CC3**	T	-5.10	0.92	-5.88	-5.06	-2.10	0.86	3.82	6.78
5CH_4@**CC3**	C_1	-5.11	0.92	-5.87	-4.65	-2.24	0.17	2.58	4.99
6CH_4@**CC3**	T	-1.98	0.96	-1.32	-0.71	2.31	5.33	8.35	11.37
6CH_4@**CC3**	C_1	-2.00	0.96	-1.33	-0.01	2.87	5.74	8.74	11.49
CH_4@**CC3**	T	-3.02	0.73	-5.24	-5.79	-4.33	-2.86	-1.40	0.07
CO_2@**CC3**-a	C_3	-6.06	1.42	-8.88	-9.18	-7.30	-5.42	-3.54	-1.66
CO_2@**CC3**-b	C_2	-7.02	1.81	-6.51	-5.51	-3.13	-0.75	1.62	4.00
4CO_2@**CC3**-a	C_2	-7.57	1.70	-8.46	-7.69	-4.80	-1.91	0.98	3.88
4CO_2@**CC3**-b	C_1	-8.63	1.67	-8.43	-7.51	-4.45	-1.40	1.65	4.70
6CO_2@**CC3**-a	T	-6.65	1.86	-5.65	-5.42	-1.97	1.49	4.95	8.40
6CO_2@**CC3**-b	C_3	-8.29	1.71	-7.86	-7.15	-3.87	-0.58	2.71	6.00
6CO_2@**CC3**-c	C_1	-8.97	1.66	-8.64	-7.73	-4.49	-1.26	1.97	5.20

$(CO_2)_4$[e]	S_4	-2.88	1.37	-1.34	-0.72	1.04	2.80	4.56	6.33
$(CO_2)_6$-a[e]	T_h	-3.08	0.91	-2.45	-1.75	0.49	2.74	4.98	7.22
$(CO_2)_6$-b[e]	C_1	-3.47	0.91	-2.40	-1.68	0.52	2.73	4.94	7.12
$(CO_2)_6$-c[e]	S_6	-3.85	0.74	-2.97	-2.26	0.04	2.34	4.64	6.94
(C_2H_2)@**CC3**	C_3	-5.67	1.63	-7.08	-6.14	-4.27	-2.39	-0.52	1.35
$(C_2H_2)_4$@**CC3**	C_2	-7.82	1.49	-9.70	-8.62	-5.73	-2.85	0.04	2.93
$(C_2H_2)_6$@**CC3**	C_3	-3.28	1.49	-3.98	-3.15	-0.09	2.96	6.01	9.07
$(C_2H_2)_4$[f]	S_4	-2.35	0.56	-2.35	-2.01	-0.25	1.50	3.26	5.02
$(C_2H_2)_4$[f]	C_1	-2.35	0.55	-2.42	-1.76	-0.19	1.38	2.95	4.52
$(C_2H_2)_6$[f]	C_3	-2.39	0.74	-3.01	-2.26	-0.37	1.52	3.41	5.30
H_2O@**CC3**	C_1	-12.94	3.14	-11.52	-9.44	-6.76	-4.08	-1.40	1.28
$6H_2O$@**CC3**	C_1	-16.83	1.31	-17.00	-15.11	-11.65	-8.20	-4.75	-1.29
$8H_2O$@**CC3**	C_1	-17.13	1.27	-17.19	-15.35	-11.70	-8.05	-4.40	-0.76
$12H_2O$@**CC3**	C_3	-18.53	1.54	-18.31	-16.35	-12.62	-8.89	-5.16	-1.43
$(H_2O)_6$[g]	C_1	-12.38	1.84	-11.25	-9.54	-6.85	-4.15	-1.45	1.24
$(H_2O)_8$[g]	D_{2d}	-14.28	1.87	-13.53	-11.79	-8.82	-5.86	-2.89	0.08
$(H_2O)_{12}$[g]	D_3	-14.60	1.71	-14.04	-12.29	-9.19	-6.09	-2.09	0.11
(**CC3**-*R*)$_2$ w-to-w[b]	D_3	-25.17	7.64	-33.95	-32.28	-26.39	-20.50	-14.61	-8.72
(**CC3**-*R*)$_2$ w-to-a[b]	C_3	-20.75	5.06	-30.27	-29.21	-25.31	-21.41	-17.51	-13.62
(**CC3**-*R*)$_2$ a-to-a[b]	D_3	-14.19	5.26	-23.08	-24.02	-20.20	-16.37	-12.55	-8.72
CC3-*R*/*S* w-to-w[b]	S_6	-29.41	7.26	-39.75	-38.03	-33.12	-28.21	-23.30	-18.39
Xe@w-to-w-a[c]	C_3	-8.13	2.44	-10.97	-10.47	-8.72	-6.96	-5.21	-3.46
Xe@w-to-w TS	C_3	-6.38	1.87	-9.39	-10.01	-7.46	-4.91	-2.36	0.19
Xe@w-to-w-b[d]	D_3	-7.44	1.87	-10.86	-10.54	-8.52	-6.49	-4.47	-2.44
3Xe@w-to-w	D_3	-8.06	1.89	-10.74	-10.45	-8.38	-6.31	-4.25	-2.18
Xe@w-to-w(*R*/*S*)	S_6	-8.22	2.01	-11.51	-11.35	-9.44	-7.53	-5.62	-3.71
Diphenylether	C_2								
Dimesitylether	C_2								
Octachloropropane	C_{2v}								
Hexachloropropene	C_s								
Benzylbenzoate	C_1								
Tetrachloroethene	D_{2h}								
15-Crown-5[i]	D_5	10.90		8.47	6.35	8.59	10.83	13.08	15.32
15-Crown-5[i]	C_1	0.00		0.00	0.00	0.00	0.00	0.00	0.00
Mesitylene	C_{3v}								
$HCCl_3$@**CC3**	C_1	-11.35	2.27	-16.70	-15.34	-12.41	-9.48	-6.55	-3.62
Diphenylether@**CC3**	C_2	-12.74	6.34	-13.73	-12.61	-7.01	-1.40	4.21	9.82
Dimesitylether@**CC3**	C_2	19.61	7.71	14.51	16.58	24.25	31.91	39.58	47.24
Octachloropropane@**CC3**	C_1	4.73	4.54	0.90	1.15	6.40	11.66	16.91	22.17
Hexachloropropene@**CC3**	C_1	-10.44	4.26	-14.92	-14.04	-9.10	-4.16	0.78	5.72
Benzylbenzoate@**CC3**-a	C_1	-20.02	6.66	-25.82	-24.58	-18.97	-13.35	-7.73	-2.11
Benzylbenzoate@**CC3**-b	C_1	-20.69	6.68	-24.65	-23.30	-17.69	-12.07	-6.46	-0.84
Tetrachloroethene@**CC3**	C_1	-10.19	2.82	-13.83	-12.74	-9.07	-5.41	-1.74	1.92
15-Crown-5@**CC3**	C_1	2.84	7.88	2.29	4.08	9.93	15.78	21.63	27.49
Mesitylene@**CC3**	C_3	-16.79	4.55	-23.29	-23.27	-18.55	-13.83	-9.11	-4.40
Mesitylene@**CC3**	C_1	-17.44	4.59	-22.99	-21.87	-17.54	-13.22	-8.89	-4.57
Mesitylene@**CC3**-TS	C_1	5.12	4.48	2.51	3.47	8.92	14.37	19.82	25.27
5-^{t}Bu-*m*-xylene@**CC3**	C_1	-17.24	5.81	-20.82	-19.36	-13.56	-7.76	-1.95	3.85
CC3-*R*-a(+)[j]	D_2	184.68	0.00	164.42	158.84	157.99	157.13	156.27	155.41

CC3-*R*-b(+)[j]	C_2	183.98	0.00	165.70	162.73	162.38	162.02	161.66	161.30
3I@**CC3**-a	C_2	-2.62	1.30	-6.12	-5.77	-4.26	-2.75	-1.23	0.28
3I@**CC3**-b	C_1	-3.50	1.31	-7.47	-6.95	-5.52	-4.09	-2.66	-1.23
5I@**CC3**	C_2	-4.74	1.14	-8.92	-8.47	-6.93	-5.39	-3.85	-2.32
7I@**CC3**	C_1	-5.32	1.02	-9.04	-8.60	-7.05	-5.49	-3.94	-2.38
9I@**CC3**	C_2	-5.49	0.93	-8.88	-8.45	-6.88	-5.32	-3.75	-2.18
I_2	D_{ih}	0.0	0.00	0.00	0.00	0.00	0.00	0.00	0.00
I_3	D_{ih}	5.43	0.00	2.13	2.39	2.97	3.55	4.13	4.71
$I_3(-)$	D_{ih}	-32.85	0.00	-33.88	-33.73	-32.28	-32.83	-32.37	-31.92
I_5	C_1	1.16	0.00	-0.28	-0.08	0.45	0.99	1.52	2.05
$I_5(-)$	C_{2v}	-24.53	0.00	-24.29	-24.28	-24.11	-23.95	-23.78	-23.61
I_7	C_1	-0.08	0.00	-1.33	-1.05	-0.28	0.50	1.28	2.06
$I_7(-)$	C_{3v}	-18.47	0.00	-19.63	-19.36	-18.52	-17.68	-16.84	-16.00
I_9	C_2	-0.80	0.00	-1.96	-1.64	-0.73	0.19	1.11	2.03
$I_9(-)$	T_d	-15.43	0.00	-16.51	-16.20	-15.31	-14.43	-13.54	-12.66

a) All species are optimized at the M06-2X/6-31G(d) level. Values are on a per enclosed atom or per enclosed molecule basis. For iodine-containing species, the values are per iodine atom but the reference is relative to the number of I_2 units (i.e. 1/9 of the reactions $4.5I_2$ + **CC3** → 9I@**CC3** and $4.5I_2 \rightarrow I_9(-)$). The Kr/Xe/I atoms were described with the small-core Stuttgart pseudopotential (SDD(Kr/Xe/I)) at the M06-2X/6-31G(d) and B3LYP-D3BJ/6-31G(d,p) levels.

b) Thermodynamic values for the dimerization of two units of **CC3**.

c) Xe is in the intrinsic cavity (side cavity).

d) Xe is in the extrinsic cavity (middle cavity).

e) Binding of cluster on a per CO_2 molecule basis.

f) Binding of cluster on a per C_2H_2 molecule basis

g) Binding of cluster on a per H_2O molecule basis.

h) Binding of cluster on a per SF_6 molecule basis

i) Thermodynamic values for D_5-symmetry structure of 15-crown-5 relative to the C_1-symmetry structure.

j) Thermodynamic values for **CC3**-*R*(+) radical cation are relative to neutral **CC3**-*R*. The D_2-symmetry species had one imaginary frequency which lead to a C_2-symmetry species 0.7 kcal/mol lower in energy at the M06-2X/6-31G(d) level. However, the D_2-symmetry species was 3.9 kcal/mol more stable in enthalpy (298K) at the standard level of theory.

Table S2. Point Groups, Absolute Energies (Hartrees) , Zero-Point Energies (kcal/mol), Number of Imaginary Frequencies, Capacity Corrections (kcal/mol) , and Entropies (cal/mol-K) for Various Species

	PG	label	M06-2X/6-31G(d)					B3LYP/6-31G(d,p)-D3BJ //M06-2X/6-31G(d)
			E	ZPE(NIF)	Cp(298K)	S		E
CH_4	T_d	cc3-ch4	-40.482038	28.65(0)	2.39	44.46		-40.525925
$HCCl_3$	C_{3v}	cc3-hccl3	-1419.164297	12.84(0)	3.35	70.38		-1419.290168
Xe	K	cc3-xe	-15.478947	0.00(0)	1.48	40.54		-15.539459
Kr	K	cc3-kr	-18.335064	0.00(0)	1.48	39.20		-18.393871
CO_2	D_{ih}	cc3-co2	-188.509012	7.47(0)	2.24	51.08		-188.582410
C_2H_2	D_{ih}	cc3-rcc	-77.287780	17.18(0)	2.35	47.79		-77.331811
H_2O	C_{2v}	cc3-h2o	-76.373394	13.52(0)	2.37	45.11		-76.420301
SF_6	O_h	cc3-sf6	-996.886328	13.73(0)	4.05	69.82		-997.113170
15-Crown-5	D_5	crown4	-768.797011	197.23(4)	8.15	101.44		-769.209431
15-Crown-5	C_1	crown22	-768.814389	197.32(0)	10.18	123.87		-769.222922
Mesitylene	C_{3v}	cc3-mes2	-350.026733	116.22(0)	6.74	96.09		-350.254567
5-^{t}Bu-*m*-xylene	C_s	cc3-dpe10	-467.907245	170.35(0)	9.01	114.94		-468.219820
CC3-R	T	cc3-r	-3449.811797	920.39(0)	45.99	378.78		-3451.781546
Xe@**CC3**	T	cc3-xex	-3465.303060	920.51(0)	47.68	401.59		-3467.341808
3Xe@**CC3**	C_3	cc3-rcj	-3496.279406	920.86(0)	50.76	435.50		-3498.446400
4Xe@**CC3**	T	cc3-rc	-3511.769899	920.53(3)	50.80	455.08[a]		-3514.001263
4Xe@**CC3**	C_1	cc3-rcx	-3511.770034	921.20(0)	52.30	452.50		-3514.001264
5Xe@**CC3**	T	cc3-xexx	-3527.253181	921.51(3)	52.11	462.54[a]		-3529.551781
5Xe@**CC3**	C_1	cc3-xexxqq	-3527.253376	921.92(0)	53.73	470.72		-3529.551652
Kr@**CC3**	T	cc3-krx	-3468.153873	920.61(0)	47.58	395.27		-3470.188150
4Kr@**CC3**	T	cc3-re	-3523.180444	920.74(0)	52.49	447.99		-3525.401513
5Kr@**CC3**	T	cc3-krxx	-3541.517783	921.25(0)	54.07	469.43		-3543.802298
SF_6@**CC3**-TS	C_3	cc3-rsf6ts	-4446.704542	934.20(3)	49.32	421.07[b]		-4448.908850
SF_6@**CC3**-TS	C_1	cc3-rsf6ty	-4446.707802	934.70(1)	50.29	419.36		-4448.912943
SF_6@**CC3**	T	cc3-rsf6c	-4446.713646	934.24(0)	50.99	425.13		-4448.926350
4SF_6@**CC3**	T	cc3-rsf6by	-7437.416486	978.51(0)	64.34	512.21		-7440.334772
5SF_6@**CC3**	T	cc3-rsf6bx	-8434.323681	992.27(3)	67.62	570.11[a]		-8437.490427
5SF_6@**CC3**	C_3	cc3-rsf6bxx	-8434.325076	992.95(0)	69.09	558.01		-8437.487444
$(SF_6)_4$	T	cc3-sf6bby	-3987.551264	55.27(0)	19.29	237.77		-3988.463895
$(SF_6)_5$	D_2	cc3-sf6bb	-4984.447231	69.70(1)	23.22	267.16[a]		-4985.587925
$(SF_6)_5$	C_2	cc3-sf6bbx	-4984.447462	69.94(0)	23.61	257.46		-4985.587925
CH_4@**CC3**	T	cc3-raa	-3490.298654	949.70(3)	47.17	408.59[a]		-3492.316986
CH_4@**CC3**	C_3	cc3-raax	-3490.300842	949.91(0)	48.80	406.60		-3492.317898
3CH_4@**CC3**	C_3	cc3-rbb	-3571.280207	1008.90(0)	54.01	445.65		-3573.392710
4CH_4@**CC3**-a	T	cc3-ra	-3611.769049	1037.98(6)	53.68	471.76[a]		-3613.930046
4CH_4@**CC3**-b	T	cc3-rb	-3611.769721	1038.79(0)	56.46	461.18		-3613.929442
5CH_4@**CC3**	T	cc3-raaq	-3652.262628	1069.08(3)	56.57	469.44[a]		-3654.465330
5CH_4@**CC3**	C_1	cc3-raarr	-3652.262705	1069.18(0)	58.48	480.64		-3654.465212
6CH_4@**CC3**	T	cc3-roo	-3692.722974	1099.87(6)	56.40	464.24[a]		-3694.958912
6CH_4@**CC3**	C_1	cc3-rooxx	-3692.723177	1101.24(0)	59.29	473.11		-3694.958966
CO_2@**CC3**-a	C_3	cc3-rco2	-3638.330464	928.04(2)	47.75	411.06[a]		-3640.380371
CO_2@**CC3**-b	C_2	cc3-rj0	-3638.332003	928.56(0)	48.54	406.08		-3640.377217

$4CO_2$@**CC3**-a	C_2	cc3-rjj	-4203.896077	952.80(1)	55.53	467.48[a]		-4206.175999
$4CO_2$@**CC3**-b	C_1	cc3-rj	-4203.902830	953.08(0)	55.82	461.01		-4206.175562
$6CO_2$@**CC3**-a	T	cc3-rjjj	-4580.929456	969.16(6)	56.88	477.92[a]		-4583.347875
$6CO_2$@**CC3**-b	C_3	cc3-rtt	-4580.945124	969.72(2)	59.17	487.96[a]		-4583.367497
$6CO_2$@**CC3**-c	C_1	cc3-rt	-4580.951602	969.79(0)	60.35	491.29		-4583.374558
$(CO_2)_4$	S_4	cc3-rjjx	-754.054402	31.43(0)	9.85	133.80		-754.346893
$(CO_2)_6$-a	T_h	cc3-rjjjx	-1131.083530	47.36(0)	15.07	171.85		-1131.526607
$(CO_2)_6$-b	C_1	cc3-rtx	-1131.087289	47.76(0)	14.82	174.10		-1131.526174
$(CO_2)_6$-c	S_6	cc3-rtxx	-1131.090894	47.85(0)	14.72	168.55		-1131.529972
(C_2H_2)@**CC3**	C_3	rco2cc	-3527.108606	937.99(0)	48.87	407.84		-3529.127246
$(C_2H_2)_4$@**CC3**	C_2	rjjcc	-3759.012780	993.20(0)	55.60	454.46		-3761.180088
$(C_2H_2)_6$@**CC3**	C_3	rjjjcc	-3913.569792	1028.70(0)	59.87	482.32		-3915.824648
$(C_2H_2)_4$	S_4	rjjccx	-309.166079	70.31(2)	9.17	120.85		-309.345810
$(C_2H_2)_4$	C_1	rjjccy	-309.166371	70.68(0)	10.07	128.38		-309.346166
$(C_2H_2)_6$	C_3	rjjjccx	-463.754526	106.25(0)	15.41	173.24		-464.026688
H_2O@**CC3**	C_1	cc3-ww00	-3526.205816	936.54(0)	47.81	397.07		-3528.225206
$6H_2O$@**CC3**	C_1	cc3-www	-3908.213104	1018.17(0)	54.91	442.16		-3910.478440
$8H_2O$@**CC3**	C_1	cc3-wwb	-4061.017381	1051.69(0)	56.57	447.89		-4063.379253
$12H_2O$@**CC3**	C_3	cc3-wwc	-4366.646886	1118.94(0)	61.63	472.42		-4369.204766
$(H_2O)_6$	C_1	cc3-www1	-458.358758	96.69(0)	8.91	108.83		-458.647013
$(H_2O)_8$	D_{2d}	cc3-wwb1	-611.169245	129.76(0)	11.32	123.60		-611.558716
$(H_2O)_{12}$	D_3	cc3-wwc1	-916.759862	194.39(0)	17.38	169.53		-917.344922
(**CC3**-R)$_2$ w-to-w	D_3	cc3-rdim	-6899.663698	1842.48(0)	91.95	698.66		-6903.629369
(**CC3**-R)$_2$ w-to-a	C_3	cc3-rdim6	-6899.656664	1841.18(0)	92.65	718.58		-6903.619398
(**CC3**-R)$_2$ a-to-a	D_3	cc3-rdim9	-6899.646206	1840.25(2)	91.57	719.31[a]		-6903.608255
CC3-R/S w-to-w	S_6	cc3-rdim4	-6899.670462	1842.22(0)	92.27	708.47		-6903.638014
Xe@w-to-w-a	C_3	cc3-rdim33	-	1842.76(0)	93.65	721.67		-6919.190198
Xe@w-to-w TS	C_3	cc3-rdim10	-6915.152814	1842.22(1)	93.07	713.68		-6919.186775
Xe@w-to-w-b	D_3	cc3-rdim2	-6915.154499	1842.59(0)	93.64	718.94		-6919.189116
3Xe@w-to-w	D_3	cc3-rdim3	-6946.139084	1842.85(0)	96.91	758.29		-6950.308158
Xe@w-to-w (R/S)	S_6	cc3-rdim5	-6915.162510	1842.21(0)	93.93	729.92		-6919.199030
(**CC3**-R)$_2$ w-to-w	D_3	cc3-rdim	-6899.663698	1842.48(0)	91.95	698.66		-6903.629369
Diphenlyether	C_2	cc3-dpe	-538.281307	117.77)(0)	6.79	99.51		-538.574393
Dimesitylether	C_2	cc3-dpe2	-774.064104	223.32(0)	13.14	145.91		-774.531358
Octachloropropane	C_{2v}	cc3-dpe4	-3795.527670	17.40(0)	8.40	112.01		-3795.846681
Hexachloropropene	C_s	cc3-dpe6	-2875.200045	15.53(0)	6.83	102.47		-2875.454120
Benzylbenzoate	C_1	cc3-dpe8	-690.887714	143.00(0)	8.80	119.32		-691.253809
Tetrachloroethene	D_{2h}	cc3-dpe12	-1916.796865	9.99(0)	4.62	81.12		-1916.966755
Mesitylene	C_{3v}	cc3-mes2	-350.026733	116.22(0)	6.74	96.09		-350.254567
$HCCl_3$@**CC3**	C_1	cc3-rccl33	-4868.994180	933.97(0)	49.96	419.84		-4871.101958
Diphenlyether@**CC3**	C_2	cc3-dpe1	-3988.113402	1039.58(0)	52.49	422.22		-3990.387932
Dimesitylether@**CC3**	C_2	cc3-dpe3	-4223.844652	1147.44(0)	57.48	448.04		-4226.302068
Octachloropropane@**CC3**	C_1	cc3-dpe5	-7245.331934	938.08(0)	54.35	438.23		-7247.634032
Hexchloropropene@**CC3**	C_1	cc3-dpe77	-6325.028477	936.66(0)	52.97	431.85		-6327.266234
Benzylbenzoate@**CC3**-a	C_1	cc3-dpe9	-4140.731410	1064.83(0)	54.59	441.92		-4143.087122
Benzylbenzoate@**CC3**-b	C_1	cc3-dpe999	-4140.732484	1064.98(0)	54.55	441.95		-4143.085287
Tetrachloroethene@**CC3**	C_1	cc3-dpe133	-5366.624901	931.06(0)	51.03	423.24		-5368.774839
15-Crown-5@**CC3**	C_1	cc3-crown	-4218.621655	1120.14(0)	55.53	444.13		-4221.013366

Mesitylene@**CC3**	C_3	cc3-mes3	-3799.865290	1038.01(2)	51.36	427.70[a]		-3802.080482
Mesitylene@**CC3**	C_1	cc3-mes4	-3799.866330	1038.45(0)	51.85	420.35		-3802.039252
Mesitylene@**CC3**-TS	C_1	cc3-mes3tu	-3799.830374	1037.87(1)	52.60	431.62		-3802.080071
5-^{t}Bu-*m*-xylene@**CC3**	C_1	cc3-dpe11	-3917.746511	1092.73(0)	54.47	435.68		-3920.043811
CC3-*R*-a(+)	D_2	cc3-rrad	-3449.517481	914.35(1)	46.46	387.36		-3451.519526
CC3-*R*-b(+)	C_2	cc3-raddx	-3449.518599	917.49(1)	45.93	382.35		-3451.517485
3I@**CC3**-a	C_2	cc3-i3a	-3483.919368	921.77(1)	49.78	427.30[a]		-3486.074115
3I@**CC3**-b	C_1	cc3-i3	-3483.923558	921.52(0)	50.49	429.78		-3486.080652
5I@**CC3**	C_2	cc3-i5	-3506.674608	921.94(0)	53.46	458.41		-3508.956855
7I@**CC3**	C_1	cc3-i7	-3529.426210	922.52(0)	56.42	489.04		-3531.826996
9I@**CC3**	C_2	cc3-i9a	-3552.175669	923.04(0)	59.43	519.48		-3554.693533
I_2	D_{ih}	cc3-i5c	-22.730028	0.28(0)	2.43	62.61		-22.838062
I_3	D_{ih}	cc3-i3c	-34.069074	1.34(0)	3.51	76.53		-34.246902
I_3(-)	D_{ih}	cc3-i3b	-34.252091	0.51(0)	3.98	80.29		-34.419048
I_5	C_1	cc3-i5aa	-56.815849	0.85(0)	6.43	129.82		-57.097419
I_5(-)	C_{2v}	cc3-i5b	-57.011325	1.01(0)	6.78	121.33		-57.290934
I_7	C_1	cc3-i7c	-79.555973	1.39(0)	10.00	164.72		-79.948025
I_7(-)	C_{3v}	cc3-i7b	-79.761107	1.48(0)	9.91	160.42		-80.152226
I_9	C_s	cc3-i9c	-102.296586	1.91(0)	13.08	199.14		-102.799332
I_9(-)	T_d	cc3-i9b	-102.506448	1.91(0)	13.08	202.08		-103.008068

a) The structure had one or more imaginary frequencies which were not included for the calculation of zero-point energy, heat capacity correction or entropy. The entropy value in this table was increased by an amount equal to the contribution the imaginary frequencies would make if they were real.

b) The transition state is expected to have one imaginary frequency. The entropy value for this structure was increased by an amount equal to the contribution of two imaginary frequencies would make if they were real.