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

Azide Addition to $Sc_2@C_{66}$: Favorable Activity on Unsaturated Linear Triquinanes and Dramatic Reactivity Difference Compared with Free C_{66} Cage

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Electronic Supporting Information

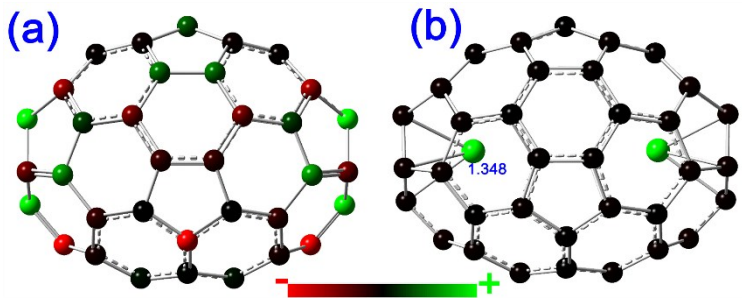

Figure S1. Natural bond orbital (NBO) analyses for free C_{66} (a) and $Sc_2@C_{66}$ (b).

Table S1. Orbital energy gaps of the frontier orbitals of CH_3N_3 and C_{66}, $Sc_2@C_{66}$.

Structure	E_{HOMO} (eV)	E_{LUMO} (eV)
CH_3N_3	-8.39	0.75
C_{66}	-6.66	-3.79
$Sc_2@C_{66}$	-6.26	-3.55

The calculations indicate that the energy difference between the LUMOs of free C_{66}, $Sc_2@C_{66}$ and the HOMO of CH_3N_3, [namely $|E_{LUMO}(C_{66}, Sc_2@C_{66}) - E_{HOMO}(CH_3N_3)|$] (4.60, 4.84 eV), is smaller than the energy gap between the HOMO of free C_{66}, $Sc_2@C_{66}$ and the LUMO of CH_3N_3, [that is $|E_{HOMO}(C_{66}, Sc_2@C_{66}) - E_{LUMO}(CH_3N_3)|$] (7.41, 7.01 eV).

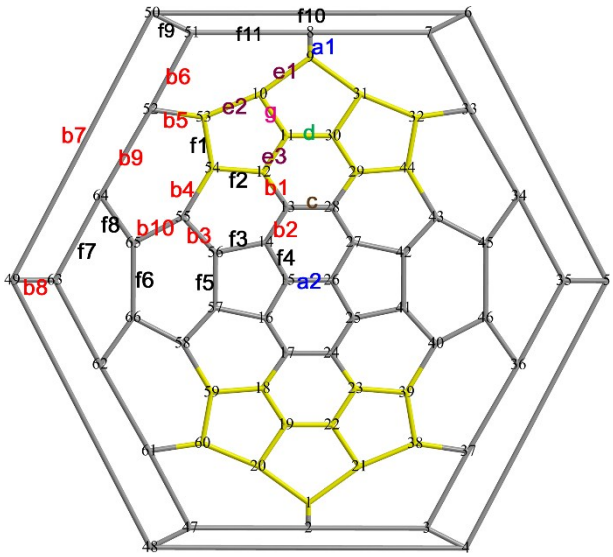

Figure S2. Representation of 29 non-equivalent C_m–C_n bonds of C_{2v}(4059)-C_{66} cage ($_m$ and $_n$ represent the atomic numbers).

Table S2. Reaction energies (ΔE_r, kcal mol^{-1}) on 29 non-equivalent C–C bonds for the two bonding types of methyl azide additions to free C_{66} and $Sc_2@C_{66}$.

Bond	Bond type	$CH_3N–C_m$	ΔE_r		$CH_3N–C_n$	ΔE_r	
		$–C_n–N–N$	C_{66}	$Sc_2@C_{66}$	$–C_m–N–N$	C_{66}	$Sc_2@C_{66}$
d	D[5,6]-55	30–11	**-40.8**	1.6 [1.1][a]	11–30	-40.7	1.4
a1	A[6,6]-55	9–8	-30.1	**-6.9** [-6.6]	8–9	-29.5	-6.2
a2	A[6,6]-55	26–15	-24.2	-2.3 [-3.2]	15–26	-24.2	-2.0
b1	B[6,6]-56	12–13	-12.3	3.7 [3.9]	13–12	-12.1	3.4
b2	B[6,6]-56	13–14	-17.1	-12.3 [-12.0]	14–13	-16.9	-11.4
b3	B[6,6]-56	55–56	-6.2	-4.7 [-4.3]	56–55	-6.9	-4.6
b4	B[6,6]-56	54–55	-9.2	11.7 [11.8]	55–54	-8.5	10.7
b5	B[6,6]-56	53–52	2.6	-2.6 [-2.7]	52–53	3.4	-2.8
b6	B[6,6]-56	52–51	-8.9	-5.2 [-5.2]	51–52	-4.4	-4.8
b7	B[6,6]-56	49–50	-4.6	1.7 [1.9]	50–49	-4.4	4.0
b8	B[6,6]-56	49–63	-1.1	0.7 [1.3]	63–49	-0.4	0.9
b9	B[6,6]-56	52–64	-14.9	-7.6 [-6.4]	64–52	-15.0	-6.5
b10	B[6,6]-56	55–65	7.1	-2.6 [-2.8]	65–55	7.6	-2.6
c	C[6,6]-66	28–13	5.8	5.3 [4.3]	13–28	5.8	5.2
e1	E[5,6]-56	9–10	-23.3	**-6.4** [-6.6]	10–9	-22.8	-6.6
e2	E[5,6]-56	10–53	**-44.4**	-4.1 [-3.9]	53–10	-44.1	-3.7
e3	E[5,6]-56	11–12	-19.0	-13.9 [-11.9]	12–11	-18.2	-14.8
f1	F[5,6]-66	54–53	-4.7	-14.2 [-14.4]	53–54	-5.8	-14.7
f2	F[5,6]-66	54–12	-28.4	-4.0 [-4.9]	12–54	-29.4	-4.6
f3	F[5,6]-66	56–14	-16.6	-1.8 [0.9]	14–56	-16.2	-1.4
f4	F[5,6]-66	14–15	-0.2	-6.1 [-7.4]	15–14	-0.8	-7.7
f5	F[5,6]-66	56–57	-11.6	**-16.1** [-15.8]	57–56	-11.7	-16.1
f6	F[5,6]-66	65–66	-34.7	-13.9 [-12.1]	66–65	-34.6	-14.0
f7	F[5,6]-66	63–64	-18.6	-9.3 [-9.2]	64–63	-17.8	-7.3
f8	F[5,6]-66	64–65	-19.3	-4.7 [-2.8]	65–64	-18.7	-5.4
f9	F[5,6]-66	50–51	-30.3	-13.8 [-12.6]	51–50	-30.9	-14.2
f10	F[5,6]-66	6–50	-17.1	2.5 [1.5]	50–6	-17.1	2.8
f11	F[5,6]-66	8–51	-13.0	-7.4 [-8.4]	51–8	-14.3	-7.8
g	G[5,5]-66	11–10	-31.4	**-16.0** [-14.0]	10–11	-31.0	-15.9

[a] Single-point energy calculations upon the optimized structures involving solvent effect ortho-dichlorobenzene (ODCB) are performed by the polarizable continuum model (PCM).

Table S3. Energy barriers ($\Delta E^{\neq}$, kcal mol^{-1}) on 29 non-equivalent C–C bonds for 1,3-dipolar cycloaddition of methyl azide to free C_{66} and $Sc_2@C_{66}$. The values considering solvent ODCB are presented in brackets.

Bond	Bond type	C_m–C_n	C_{66}	$Sc_2@C_{66}$
d	D[5,6]-55	30–11	**3.4**	23.3 [23.3]
a1	A[6,6]-55	9–8	8.7	**19.1** [19.1]
a2	A[6,6]-55	26–15	10.8	22.8 [22.7]
b1	B[6,6]-56	12–13	18.6	24.5 [24.9]
b2	B[6,6]-56	13–14	16.6	20.0 [21.5]
b3	B[6,6]-56	55–56	21.2	22.8 [24.6]
b4	B[6,6]-56	54–55	18.7	31.6 [32.7]
b5	B[6,6]-56	53–52	18.5	24.3 [23.9]
b6	B[6,6]-56	52–51	27.9	22.1 [23.5]
b7	B[6,6]-56	49–50	22.8	25.9 [27.1]
b8	B[6,6]-56	49–63	23.3	24.6 [25.9]
b9	B[6,6]-56	52–64	17.1	22.0 [23.2]
b10	B[6,6]-56	55–65	28.4	24.0 [24.6]
c	C[6,6]-66	28–13	26.3	26.2 [27.0]
e1	E[5,6]-56	9–10	13.6	**19.0** [19.1]
e2	E[5,6]-56	10–53	**6.7**	22.9 [22.8]
e3	E[5,6]-56	11–12	11.4	20.5 [20.5]
f1	F[5,6]-66	54–53	25.3	20.8 [21.1]
f2	F[5,6]-66	54–12	12.5	24.2 [24.2]
f3	F[5,6]-66	56–14	16.2	26.5 [29.3]
f4	F[5,6]-66	14–15	25.5	26.3 [25.9]
f5	F[5,6]-66	56–57	20.1	**22.2** [22.2]
f6	F[5,6]-66	65–66	10.9	22.8 [25.5]
f7	F[5,6]-66	63–64	20.5	23.0 [23.8]
f8	F[5,6]-66	64–65	20.2	25.9 [28.3]
f9	F[5,6]-66	50–51	13.0	23.5 [25.2]
f10	F[5,6]-66	6–50	18.8	28.6 [30.0]
f11	F[5,6]-66	8–51	26.1	25.1 [25.4]
g	G[5,5]-66	11–10	10.9	**19.2** [19.1]

Table S4. Bond lengths (Å) of adducts and the corresponding transition states for free C_{66} and $Sc_2@C_{66}$. R_{CC} (P), R_1 (TS) and R_2 (TS) represent the bond lengths of C_m–C_n in adducts (P), C_m–NCH_3 and C_n–N in the corresponding transition states (TS), respectively.

			C_{66}			$Sc_2@C_{66}$		
Bond	Bond type	C_m–C_n	R_{CC} (P)	R_1 (TS)	R_2 (TS)	R_{CC} (P)	R_1 (TS)	R_2 (TS)
d	D[5,6]-55	30–11	1.530	1.986	2.451	1.600	1.800	2.201
a1	A[6,6]-55	9–8	1.555	1.945	2.410	1.582	1.812	2.268
a2	A[6,6]-55	26–15	1.546	2.018	2.238	1.560	1.909	2.183
b1	B[6,6]-56	12–13	1.606	1.853	2.360	1.634	1.760	2.262
b2	B[6,6]-56	13–14	1.582	1.984	2.205	1.591	1.942	2.234
b3	B[6,6]-56	55–56	1.590	1.987	2.084	1.591	1.943	2.154
b4	B[6,6]-56	54–55	1.570	1.763	2.450	1.588	1.775	2.194
b5[a]	B[6,6]-56	53–52	1.593	1.611	2.366	1.605	1.804	2.286
b6	B[6,6]-56	52–51	1.604	2.070	2.175	1.632	1.901	2.175
b7	B[6,6]-56	49–50	1.575	1.982	2.096	1.584	1.887	2.184
b8	B[6,6]-56	49–63	1.606	1.921	2.137	1.602	1.916	2.134
b9	B[6,6]-56	52–64	1.571	2.011	2.173	1.584	1.886	2.266
b10	B[6,6]-56	55–65	1.590	1.918	2.043	1.594	1.935	2.158
c	C[6,6]-66	28–13	1.759	1.732	2.285	1.743	1.791	2.200
e1	E[5,6]-56	9–10	1.564	1.650	2.548	1.646	1.794	2.280
e2	E[5,6]-56	10–53	1.560	2.052	2.404	1.596	1.821	2.215
e3	E[5,6]-56	11–12	1.555	1.594	2.517	1.580	1.877	2.216
f1	F[5,6]-66	54–53	1.588	1.580	2.364	1.646	1.982	2.121
f2	F[5,6]-66	54–12	1.607	2.028	2.251	1.656	1.915	2.111
f3	F[5,6]-66	56–14	1.594	1.856	2.400	1.607	1.873	2.248
f4	F[5,6]-66	14–15	1.582	1.629	2.400	1.587	1.971	2.128
f5	F[5,6]-66	56–57	1.580	1.696	2.501	1.597	2.020	2.172
f6	F[5,6]-66	65–66	1.576	2.077	2.271	1.588	1.996	2.180
f7	F[5,6]-66	63–64	1.577	2.032	2.170	1.590	1.929	2.244
f8	F[5,6]-66	64–65	1.583	1.609	2.664	1.609	1.963	2.136
f9	F[5,6]-66	50–51	1.584	2.032	2.272	1.602	2.046	2.104
f10	F[5,6]-66	6–50	1.582	1.604	2.558	1.620	1.910	2.146
f11	F[5,6]-66	8–51	1.581	1.937	2.138	1.625	1.923	2.165
g	G[5,5]-66	11–10	1.555	1.599	2.589	1.602	1.897	2.223

[a]For TSs b5, e1, e3, f1, f4, f8, f10, and g in free C_{66}, the C_m–NCH_3 bond lengths shorten to around 1.600 Å (grey shaded part), which was also discovered in previous reports. The frequency analyses of these transition states turned out to be only one imaginary frequency and meanwhile show the concerted vibrations from H_3C–N to C_m and N to C_n. Subsequent intrinsic reaction coordinate (IRC) analyses demonstrate that the transition states indeed connect the reactants and adducts.

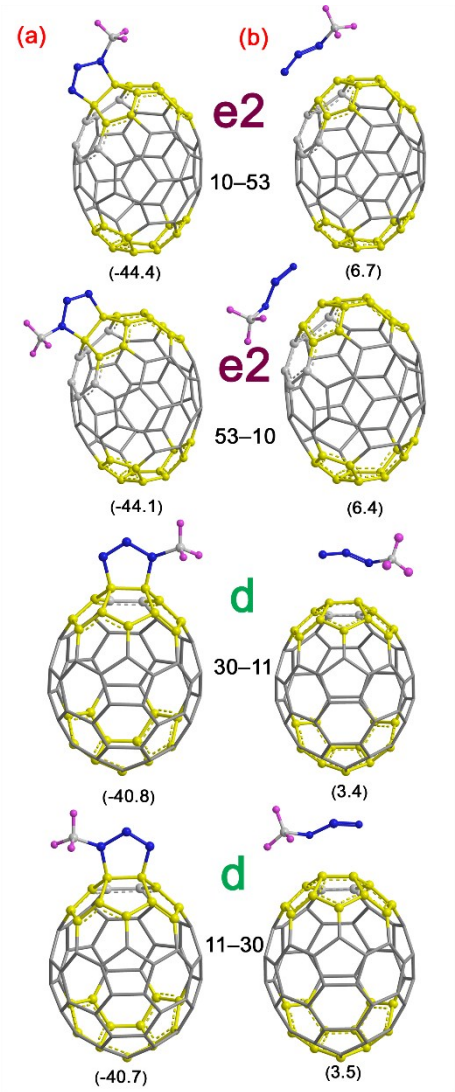

Figure S3. Structures of the adducts (a) and the corresponding transition states (b) on the most reactive sites bonds e2 and d with the two bonding types for free $C_{66.}$ The unsaturated linear triquinanes (ULTs) are colored yellow. The pink and blue balls represent H and N atoms, respectively.

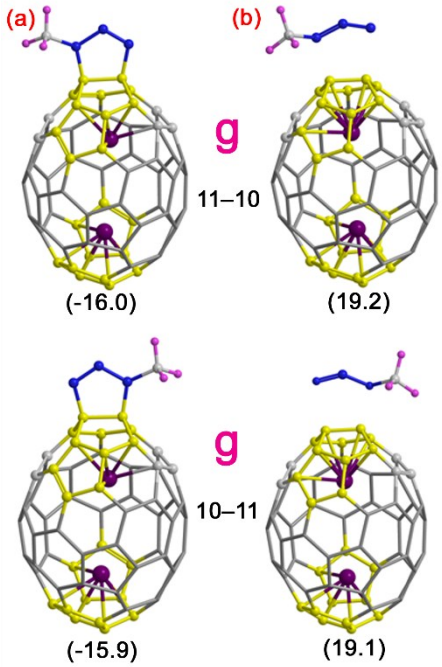

Figure S4. Structures of the adduct (a) and the corresponding transition state (b) on the most reactive site bond g with the two bonding types for $Sc_2@C_{66}$.

ref. 21 Gaussian 09, Revision A.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

Table S5. The C–C bond lengths (R, Å), NBO charges (C), and pyramidalization angles (θ_p, º) for free C_{66} and the corresponding differences between $Sc_2@C_{66}$ and C_{66} which are denoted as ΔR, ΔC and $\Delta\theta_p$, respectively.

Bond	Bond type	Bond lengths		NBO charges		POAV	
		R	ΔR	C	ΔC	θ_p	$\Delta\theta_p$
d	D[5,6]-55	1.363	0.080	0.089	-0.237	15.16	1.59
a1	A[6,6]-55	1.374	0.047	-0.001	-0.123	12.38	0.25
a2	A[6,6]-55	1.368	0.032	0.028	-0.034	11.38	-0.47
b1	B[6,6]-56	1.433	0.022	-0.025	-0.075	10.93	-0.36
b2	B[6,6]-56	1.408	0.010	-0.003	-0.072	10.05	-0.55
b3	B[6,6]-56	1.415	0.004	-0.001	-0.032	9.58	0.41
b4	B[6,6]-56	1.408	0.026	-0.009	-0.042	9.67	-0.63
b5	B[6,6]-56	1.451	-0.008	0.016	-0.088	10.36	0.42
b6	B[6,6]-56	1.443	-0.002	-0.012	-0.045	10.42	0.12
b7	B[6,6]-56	1.423	0.002	0.003	-0.033	9.57	-0.18
b8	B[6,6]-56	1.424	0.003	-0.040	0.036	10.02	-0.04
b9	B[6,6]-56	1.398	0.021	-0.008	-0.043	9.50	0.22
b10	B[6,6]-56	1.443	-0.022	-0.027	0.002	9.90	0.00
c	C[6,6]-66	1.483	-0.004	-0.002	-0.055	9.89	-0.86
e1	E[5,6]-56	1.452	0.005	0.022	-0.138	14.95	0.59
e2	E[5,6]-56	1.376	0.072	0.007	-0.144	14.21	-0.18
e3	E[5,6]-56	1.437	-0.004	0.020	-0.166	13.57	0.87
f1	F[5,6]-66	1.490	-0.048	0.033	-0.150	11.04	-0.23
f2	F[5,6]-66	1.418	0.038	-0.015	-0.107	11.25	-0.49
f3	F[5,6]-66	1.432	0.020	0.015	-0.093	10.27	0.37
f4	F[5,6]-66	1.450	-0.022	0.012	-0.061	10.80	-0.36
f5	F[5,6]-66	1.448	-0.020	0.035	-0.098	10.33	0.97
f6	F[5,6]-66	1.390	0.038	-0.017	-0.030	10.98	0.08
f7	F[5,6]-66	1.427	0.005	-0.040	-0.019	10.58	0.02
f8	F[5,6]-66	1.468	-0.025	-0.009	-0.061	10.41	0.18
f9	F[5,6]-66	1.410	0.019	-0.001	-0.090	11.04	-0.23
f10	F[5,6]-66	1.467	-0.026	0.005	-0.085	10.45	-0.48
f11	F[5,6]-66	1.455	-0.001	-0.044	-0.086	11.70	-0.83
g	G[5,5]-66	1.466	-0.016	0.027	-0.172	16.01	0.29

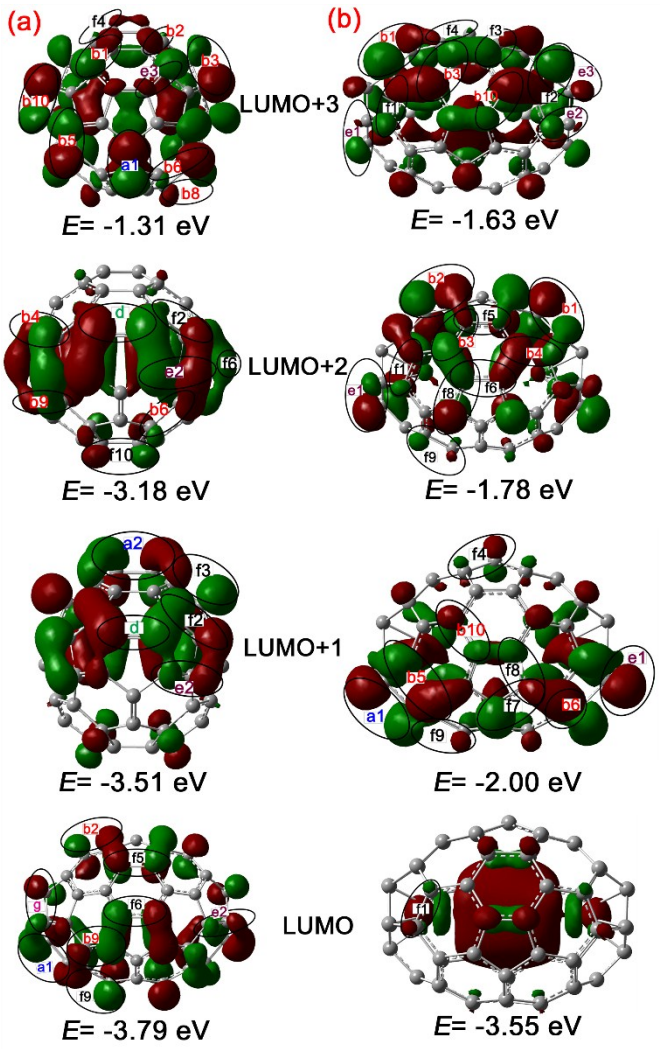

Figure S5. Representation of low-lying unoccupied molecular orbitals (iso-surface value is 0.020) of free C_{66} (a) and $Sc_2@C_{66}$ (b). Only those bonds with appropriate orbitals to interact with the HOMO of CH_3N_3 are highlighted with ellipses.

Table S6. Contributions of the appropriate unoccupied molecular orbitals for free C_{66} and $Sc_2@C_{66}$ to interact with the HOMO of CH_3N_3.

Bond	Bond type	LUMOs (C_{66})				LUMOs ($Sc_2@C_{66}$)			
		0	+1	+2	+3	0	+1	+2	+3
d	D[5,6]-55		6.96	9.17					
a1	A[6,6]-55	7.05			6.75		14.93		
a2	A[6,6]-55		9.66						
b1	B[6,6]-56				3.08			6.37	7.52
b2	B[6,6]-56	4.34			1.52			8.25	
b3	B[6,6]-56				6.84			3.29	4.79
b4	B[6,6]-56			4.09				3.84	
b5	B[6,6]-56				6.46		7.72		
b6	B[6,6]-56			2.29	3.84		4.71		
b7	B[6,6]-56								
b8	B[6,6]-56				2.06				
b9	B[6,6]-56	3.93		2.78					
b10	B[6,6]-56				7.21		1.31		4.52
c	C[6,6]-66								
e1	E[5,6]-56						9.99	3.73	1.50
e2	E[5,6]-56	1.81	3.34	7.92					1.37
e3	E[5,6]-56				2.68				7.78
f1	F[5,6]-66					1.60		2.68	2.76
f2	F[5,6]-66		6.12	3.44					7.75
f3	F[5,6]-66		6.67						1.48
f4	F[5,6]-66				0.87		1.05		0.38
f5	F[5,6]-66	3.77						1.63	
f6	F[5,6]-66	4.26		4.19				3.17	
f7	F[5,6]-66						3.68		
f8	F[5,6]-66						1.50	3.72	
f9	F[5,6]-66	5.37					0.95	0.89	
f10	F[5,6]-66			2.61					
f11	F[5,6]-66								
g	G[5,5]-66	2.46							

Table S7. Reaction energies (ΔE_r, kcal mol^{-1}) for 1,3-dipolar cycloaddition of methyl azide to 29 non-equivalent C–C bonds for C_{66}^{6-} cage.

Bond	Bond type	ΔE_r
d	D[5,6]-55	-52.5
a1	A[6,6]-55	-38.8
a2	A[6,6]-55	-26.9
b1	B[6,6]-56	-39.3
b2	B[6,6]-56	-32.4
b3	B[6,6]-56	-34.3
b4	B[6,6]-56	-28.5
b5	B[6,6]-56	-41.1
b6	B[6,6]-56	-35.0
b7	B[6,6]-56	-29.4
b8	B[6,6]-56	-27.8
b9	B[6,6]-56	-27.5
b10	B[6,6]-56	-31.0
c	C[6,6]-66	-33.0
e1	E[5,6]-56	-56.2
e2	E[5,6]-56	-47.6
e3	E[5,6]-56	-53.5
f1	F[5,6]-66	-48.6
f2	F[5,6]-66	-39.4
f3	F[5,6]-66	-37.2
f4	F[5,6]-66	-38.5
f5	F[5,6]-66	-42.3
f6	F[5,6]-66	-38.9
f7	F[5,6]-66	-38.8
f8	F[5,6]-66	-37.0
f9	F[5,6]-66	-40.5
f10	F[5,6]-66	-33.4
f11	F[5,6]-66	-38.9
g	G[5,5]-66	-65.6

Table S8. Reaction energies (ΔE_r, kcal mol^{-1}) and energy barriers ($\Delta E^{\neq}$, kcal mol^{-1}) for 1,3-dipolar cycloaddition reaction of 4-isopropoxyphenyl azide to $Sc_2@C_{66}$ including gas phase and solvent effects (ortho-dichlorobenzene).

Bond	Bond type	Gas phase		Solvent phase	
		ΔE_r	$\Delta E^{\neq}$	ΔE_r	$\Delta E^{\neq}$
d	D[5,6]-55	7.1		6.4	
a1	A[6,6]-55	-1.0		0.6	
a2	A[6,6]-55	3.9		3.0	
b1	B[6,6]-56	10.6		10.9	
b2	B[6,6]-56	-6.1		-6.0	
b3	B[6,6]-56	0.1		-2.2	
b4	B[6,6]-56	18.3		17.6	
b5	B[6,6]-56	3.6		3.5	
b6	B[6,6]-56	0.5		0.7	
b7	B[6,6]-56	7.8		6.6	
b8	B[6,6]-56	6.6		6.8	
b9	B[6,6]-56	-1.5		-2.5	
b10	B[6,6]-56	2.5		3.5	
c	C[6,6]-66	11.2		8.4	
e1	E[5,6]-56	-1.8		-1.6	
e2	E[5,6]-56	2.6		2.5	
e3	E[5,6]-56	-8.6	24.6	-6.1	24.7
f1	F[5,6]-66	-8.9	24.5	-6.9	25.3
f2	F[5,6]-66	1.8		0.9	
f3	F[5,6]-66	4.4		6.9	
f4	F[5,6]-66	0.5		-0.9	
f5	F[5,6]-66	-9.6	24.6	-8.6	26.2
f6	F[5,6]-66	-7.2	25.6	-6.2	26.6
f7	F[5,6]-66	-2.5		-3.0	
f8	F[5,6]-66	0.1		0.6	
f9	F[5,6]-66	-7.6	26.2	-6.8	26.5
f10	F[5,6]-66	7.4		6.7	
f11	F[5,6]-66	-2.3		-3.3	
g	G[5,5]-66	-12.0	22.9	-11.2	22.8

Table S9. Atom coordinates and absolute energies

S9.1 Methyl azide additions to free C_{66}

TS---d---22–19

C	1.30007800	2.42554000	2.77519800	C	-0.88901000	3.50117400	2.57138000
C	1.84676700	3.58141100	3.29053300	C	-1.66167700	3.60434800	1.30259500
C	0.99412600	4.71349000	3.60528300	C	-2.10366200	4.85912200	0.82508800
C	1.76967300	5.88689500	3.47516400	C	-2.14010900	5.02362700	-0.57406200
C	1.18392300	7.13527600	3.12817600	C	-1.99972000	6.33576800	-1.16496900
C	2.00028600	8.10178600	2.47745400	C	-1.83186800	7.48001000	-0.35007800
C	1.45061400	9.09338300	1.63781400	C	-1.15371300	8.57343500	-0.92382800
C	2.46228700	9.45257500	0.65677000	C	-1.73248900	7.28519900	1.07627300
C	2.09034600	9.92027500	-0.58226900	C	-1.86497800	6.02253800	1.64267900
C	2.76102200	9.41084100	-1.76238100	C	3.08708300	4.11073100	2.74754600
C	1.71968700	9.07264900	-2.73987900	C	3.07944300	5.50778300	2.93830800
C	1.95398800	7.75626300	-3.26359500	C	3.78095900	6.38954500	2.06592300
C	0.85588400	6.85020900	-3.44050800	C	3.31415100	7.72534100	1.94371200
C	1.19904700	5.48630300	-3.43027900	C	3.54481700	8.48907200	0.77886800
C	0.25925200	4.45058200	-3.04923000	C	4.09547700	7.86496600	-0.39761000
C	0.97376100	3.33446500	-2.46640700	C	3.60399300	8.32498300	-1.68262900
C	0.40338800	2.50248100	-1.49072800	C	3.17894200	7.32169900	-2.69870000
C	1.33286000	1.86403100	-0.60112300	C	3.45753100	5.95236400	-2.51573600
C	0.92305700	1.37990900	0.68926000	C	2.49325800	5.03576100	-3.00382700
C	1.94750500	1.77701500	1.65726200	C	2.35942300	3.72515800	-2.41849300
C	-0.12683400	2.35950400	2.52867700	C	3.17898700	3.33342400	-1.33879700
C	-0.34293900	1.70697700	1.20445800	C	2.65217600	2.36203200	-0.45761300
C	-1.19828500	2.60477000	0.42697800	C	2.98176900	2.38838700	0.98102000
C	-0.92300100	2.88912500	-0.94647600	C	3.64297000	3.55103000	1.53961700
C	-1.52249600	4.06071000	-1.44235700	C	4.27198600	4.42515700	0.64750000
C	-0.96747500	4.80590300	-2.55210800	C	4.43265800	5.81341500	0.93814100
C	-1.30038800	6.20810700	-2.41035800	C	4.48919100	6.52533900	-0.29766600
C	-0.46958000	7.23413400	-2.89859400	C	4.24579900	5.56043100	-1.37694100
C	-0.59117200	8.49168800	-2.22247200	C	4.10759200	4.29795400	-0.80718200
C	0.50057500	9.42555600	-2.24171800	N	-0.43106400	-0.81839500	1.23707800
C	0.67596500	10.00768800	-0.90825400	N	0.61443000	-1.04713700	0.84240900
C	-0.27746600	9.44492200	-0.09190800	N	-1.35809500	0.01304000	1.41725000
C	0.06089900	9.02714900	1.25676400	C	-2.13097600	-0.07167100	2.65971400
C	-0.72843400	8.03397400	1.84447700	H	-2.75188400	0.82482300	2.67645400
C	-0.21109400	7.15317900	2.84121000	H	-2.77770100	-0.95128900	2.64352200
C	-0.94461300	5.93003300	2.78297200	H	-1.48703100	-0.08397200	3.54389600
C	-0.38368900	4.71467400	3.19013900				

Gas phase Absolute energy = -2717.86411954 a.u. Zero-point corrected energy = -2717.395802 a.u.

TS---e1---9–10

C	3.79888900	2.43113900	2.88637700	C	1.62523800	3.52928100	2.55203200
C	4.39074800	3.65046700	3.13966700	C	0.79999800	3.41513500	1.31415000
C	3.57510300	4.84572000	3.26037000	C	0.37918600	4.56729700	0.62098500
C	4.37642600	5.95740100	2.87874300	C	0.28429400	4.46441800	-0.78653200
C	3.81009300	7.13142500	2.32400000	C	0.42841600	5.63794500	-1.62238200
C	4.62630300	7.92698300	1.46523700	C	0.66180000	6.90873200	-1.04630600
C	4.06552100	8.76054200	0.45396000	C	1.34129800	7.84762800	-1.84585200
C	5.03050200	8.89398700	-0.59509400	C	0.81720500	6.98882200	0.38517700
C	4.67084100	9.31634300	-1.94544100	C	0.68456000	5.85958200	1.18782200
C	5.23855800	8.42604600	-3.01812000	C	5.61372600	4.02824200	2.45184600
C	4.12950700	7.91340600	-3.82433600	C	5.64004500	5.44450900	2.36799700
C	4.30250600	6.51786400	-4.09248700	C	6.32118800	6.12378800	1.31794300
C	3.17924700	5.62779800	-4.06761700	C	5.87475900	7.42384300	0.96765500
C	3.49614700	4.28199200	-3.80781800	C	6.06987400	7.96339500	-0.34820600
C	2.54962900	3.36391700	-3.20567300	C	6.56695100	7.09903600	-1.39879200
C	3.26646800	2.35844900	-2.44594800	C	6.02526200	7.32036300	-2.72132400
C	2.71943800	1.74361400	-1.30520100	C	5.53970100	6.16072200	-3.50198100
C	3.67482000	1.24509000	-0.36008800	C	5.79801100	4.84005500	-3.08113300
C	3.30315000	1.07617200	1.02048000	C	4.79723200	3.88081400	-3.35365400
C	4.38811700	1.56491700	1.88169900	C	4.65445300	2.70838600	-2.51884100
C	2.36835600	2.37672700	2.68746200	C	5.51351000	2.50008700	-1.41353600
C	2.12193400	1.56106100	1.48890900	C	5.00986100	1.71765400	-0.35471900
C	1.20018300	2.24582100	0.62128100	C	5.39409200	2.01189600	1.05591700
C	1.42783600	2.26454400	-0.79245800	C	6.09962400	3.24242400	1.35523100
C	0.83331100	3.33896100	-1.47911500	C	6.71357000	3.91939900	0.28511000
C	1.35827900	3.84525900	-2.73376000	C	6.91726500	5.32243700	0.29844900
C	1.06262100	5.25836200	-2.84962900	C	6.93461000	5.79177600	-1.06015200
C	1.89121700	6.14637300	-3.56155600	C	6.62595000	4.65054200	-1.91856600
C	1.83486700	7.51042700	-3.12765100	C	6.48028200	3.52543700	-1.10920800
C	2.94125900	8.39551600	-3.36169700	N	5.64302300	11.01641800	-3.36421600
C	3.17975800	9.23187300	-2.19135200	N	6.01955600	10.48565800	-4.29810800
C	2.27953500	8.83077800	-1.23893400	N	5.22884900	10.85364900	-2.16384100
C	2.65303100	8.66910300	0.16252400	C	4.51092500	11.93619000	-1.49028000
C	1.86583200	7.83929400	0.95501400	H	5.11405300	12.84370200	-1.50641200
C	2.40345400	7.13865700	2.09251300	H	3.52992600	12.10426900	-1.94300400
C	1.64398900	5.95903500	2.29174800	H	4.38898400	11.59855400	-0.45971900
C	2.18792500	4.81317000	2.91031700				

Gas phase Absolute energy = -2717.84786862 a.u. Zero-point corrected energy = -2717.380194 a.u.

TS---e2---10–53

C	3.89925100	1.72359500	2.88107000	C	1.68018100	2.78209100	2.70444200
C	4.47119000	2.92999700	3.20986400	C	0.81702700	2.73924600	1.49140000
C	3.63522800	4.09672400	3.44899500	C	0.34686100	3.92888600	0.90164400
C	4.39381500	5.24127600	3.12757700	C	0.21771400	3.93450600	-0.50764900
C	3.77978600	6.44511800	2.68178500	C	0.30563400	5.17154300	-1.25255300
C	4.54215500	7.32512000	1.86454400	C	0.52467500	6.39983400	-0.58839700
C	3.92840600	8.21225500	0.95759600	C	1.15556000	7.42120700	-1.32981300
C	4.86492100	8.44591800	-0.13088500	C	0.72289300	6.36890400	0.84076600
C	4.40708300	8.77982300	-1.37679200	C	0.63846200	5.17983400	1.55688300
C	5.03159400	8.18195800	-2.57177200	C	5.66539300	3.38691600	2.51667200
C	3.89097700	7.69470700	-3.39462000	C	5.66880100	4.79843200	2.54799200
C	4.09412400	6.32699600	-3.77337000	C	6.29866200	5.56370400	1.53296800
C	2.99021700	5.41157500	-3.76687100	C	5.81460800	6.88090300	1.28061500
C	3.33375800	4.05261300	-3.63512900	C	5.96793700	7.50432000	0.02874300
C	2.42915100	3.07545600	-3.07077100	C	6.42867500	6.74570900	-1.10636000
C	3.18973800	2.03125600	-2.40807200	C	5.90430900	7.08020700	-2.42683800
C	2.68938400	1.31861800	-1.30188300	C	5.35307200	5.95663000	-3.24065600
C	3.68767500	0.77802400	-0.42759500	C	5.64375300	4.61380600	-2.92858100
C	3.36847900	0.50555600	0.94717800	C	4.65113600	3.65503700	-3.23914000
C	4.47541600	0.93831800	1.80703800	C	4.56623800	2.41323200	-2.49874800
C	2.45449400	1.64494200	2.72866200	C	5.47036100	2.14031100	-1.44537300
C	2.18558200	0.91360300	1.48853000	C	5.01575500	1.27364200	-0.43206600
C	1.22204700	1.63462100	0.70068700	C	5.44211900	1.46871000	0.98213700
C	1.40470700	1.76593500	-0.71396500	C	6.13681800	2.68778600	1.34803400
C	0.76829800	2.87696200	-1.30153000	C	6.69200500	3.45173300	0.31368800
C	1.24173400	3.48748200	-2.52676600	C	6.86687600	4.86361800	0.43237100
C	0.91673700	4.89954700	-2.52069900	C	6.83881300	5.43142300	-0.87642100
C	1.70555600	5.85989900	-3.18233600	C	6.51420400	4.34617100	-1.81064900
C	1.62727500	7.18624500	-2.64662300	C	6.43703600	3.15433200	-1.09901400
C	2.71329800	8.10406900	-2.85148600	N	7.09092600	8.93404500	-3.90024300
C	2.98083000	8.82722900	-1.60549700	N	7.70957000	7.98660800	-3.72975400
C	2.07776300	8.37769000	-0.66642000	N	6.08818900	9.62318200	-3.57977900
C	2.51508000	8.11424000	0.69048400	C	5.33220000	10.25588000	-4.66357000
C	1.77618800	7.19445800	1.44309700	H	5.87286800	11.12230900	-5.05141400
C	2.36812100	6.43414200	2.49566600	H	5.10693000	9.55529000	-5.47409200
C	1.63563300	5.21744000	2.63464100	H	4.39968300	10.59651000	-4.21127200
C	2.22643200	4.05460700	3.13859900				

Gas phase Absolute energy = -2717.85888433 a.u. Zero-point corrected energy = -2717.390992 a.u.

TS---e3---11–12

C	7.15562300	-0.09881800	6.03117300	C	5.28769300	-1.08268100	4.77377100
C	6.39086300	1.00779700	6.33092500	C	5.35509100	-1.49302700	3.34277300
C	4.97960700	1.03508200	5.98685600	C	4.42841600	-0.98811800	2.40701700
C	4.60255100	2.38939100	5.79768700	C	4.91053800	-0.77364500	1.08922200
C	3.54625500	2.75533000	4.92946900	C	4.30428200	0.21208700	0.23496600
C	3.57735900	4.05978000	4.33868700	C	3.21010700	0.99147600	0.69067400
C	2.94426500	4.33693900	3.11208800	C	3.03846600	2.25878100	0.10216200
C	3.66841200	5.42740900	2.47403800	C	2.77446000	0.80836000	2.05096500
C	3.69198300	5.53309500	1.09618100	C	3.36259500	-0.15195600	2.88018900
C	4.92081000	5.86783000	0.42203600	C	6.91573000	2.34509700	6.11040200
C	5.03666200	5.06536600	-0.87334800	C	5.81781200	3.20231900	5.86441600
C	6.34726600	4.35316500	-0.73908300	C	5.94532000	4.38010200	5.07532300
C	6.46242200	2.93841600	-0.97525500	C	4.78598000	4.87231400	4.41837700
C	7.62665800	2.34084500	-0.45624700	C	4.87566000	5.64723700	3.23285000
C	7.70384600	0.93005400	-0.14628700	C	6.13663700	5.77688700	2.55690200
C	8.63273500	0.72371400	0.94635600	C	6.10981100	5.81082100	1.10236500
C	8.49208400	-0.33287900	1.86549800	C	7.04794600	4.94793100	0.34522700
C	9.07308100	-0.10081000	3.15472900	C	8.09711700	4.28290200	1.00642600
C	8.58579900	-0.81529600	4.30449500	C	8.45281300	3.01023500	0.50337400
C	8.46954400	0.10241400	5.43949500	C	9.07332200	2.02268000	1.35846200
C	6.54715300	-1.20322200	5.32479300	C	9.32485700	2.30983000	2.72142600
C	7.45412900	-1.57186900	4.23118700	C	9.36613300	1.21127300	3.60276500
C	6.71632400	-1.68643300	3.00401100	C	8.87857200	1.34270800	5.00470000
C	7.26304800	-1.15770100	1.78625700	C	8.14502600	2.53377800	5.38570100
C	6.31561400	-0.83135800	0.80136800	C	8.25011400	3.65739600	4.55278500
C	6.56575300	0.17240900	-0.21598100	C	7.20956200	4.62649600	4.46417700
C	5.31815400	0.78763700	-0.61326500	C	7.27170400	5.23611200	3.17258000
C	5.24049000	2.11632300	-1.06247900	C	8.30523800	4.54124300	2.41001700
C	3.97743100	2.77895600	-0.85842900	C	8.89234000	3.58662100	3.23746000
C	3.88365100	4.17745600	-0.80060500	N	6.02874500	5.76374400	-2.94380200
C	3.02494200	4.53682000	0.29736300	N	7.02040200	5.20153200	-3.01118900
C	2.51357000	3.37670600	0.87499300	N	5.05343000	6.02011500	-2.15000200
C	2.40317200	3.25819100	2.31107800	C	3.78743300	6.51568600	-2.68827500
C	2.43029400	1.97152300	2.86167300	H	3.99265900	7.27914600	-3.43838100
C	2.90836100	1.72090400	4.18886700	H	3.19443700	5.69867700	-3.10771100
C	3.42124400	0.39264100	4.23543600	H	3.25139000	6.96121300	-1.84939900
C	4.42043900	0.01153900	5.15095400				

Gas phase Absolute energy = -2717.85128983 a.u. Zero-point corrected energy = -2717.383822 a.u.

TS---f1---54–53

C	5.26826000	4.24557300	5.28562300	C	2.91236900	4.81500800	5.69405400
C	5.58229900	5.57686100	5.11885000	C	1.75818700	4.28050500	4.91820700
C	4.58319300	6.60035600	5.38617000	C	0.83922000	5.14753500	4.30422400
C	4.88321300	7.72309800	4.57876700	C	0.27943500	4.72309400	3.06476900
C	3.87266300	8.61520200	4.14145800	C	-0.18164900	5.67086700	2.10686800
C	4.08926700	9.33325500	2.92510000	C	-0.09541400	7.06483900	2.35777500
C	3.02127300	9.78903400	2.13446300	C	-0.01929000	7.91804700	1.24152500
C	3.48755700	9.83212200	0.74986200	C	0.53094700	7.48523500	3.58559500
C	2.57538600	9.69285800	-0.28022300	C	0.98186900	6.55917200	4.52561100
C	2.93644000	8.80873200	-1.35003600	C	6.34313100	6.00902000	3.96100700
C	1.78768900	7.96720300	-1.70673200	C	5.97908000	7.34772600	3.68031900
C	2.19250800	6.65789000	-1.90153700	C	6.04820000	7.87784800	2.36498200
C	1.46872400	5.61841200	-1.22027700	C	5.18281500	8.95129100	2.03003000
C	2.15843900	4.42076100	-0.95028200	C	4.78080300	9.19747000	0.69435500
C	1.77572500	3.55540800	0.10346400	C	5.08535000	8.23762400	-0.33947400
C	2.94523700	2.89624600	0.66386000	C	4.10818400	8.06307400	-1.39287400
C	3.00655800	2.45876000	1.99496700	C	3.73214100	6.67854900	-1.95687800
C	4.32939800	2.36062000	2.54928200	C	4.38821700	5.53615800	-1.24667100
C	4.51699700	2.44827600	3.97147000	C	3.63391200	4.40408700	-0.97196000
C	5.67681800	3.29557600	4.26731200	C	4.09140800	3.45439000	0.00313900
C	3.92405300	3.88074500	5.68509700	C	5.30932300	3.65392400	0.69740700
C	3.48959000	2.79565300	4.79648500	C	5.41737500	3.05302400	1.97160800
C	2.18353700	3.08675600	4.27542100	C	6.18532900	3.71908100	3.05983900
C	1.88710100	2.83339700	2.89778300	C	6.60925100	5.09420200	2.88092400
C	0.83540100	3.59414800	2.35631800	C	6.61579700	5.60537300	1.57510000
C	0.71887600	3.88096000	0.94747300	C	6.43416900	6.99237900	1.30917300
C	0.07924000	5.14034700	0.77768800	C	5.87696900	7.13813700	0.00266200
C	0.36381900	5.99341900	-0.31239400	C	5.57051200	5.78702900	-0.49111100
C	0.08273400	7.38315600	-0.09166100	C	6.02999400	4.86448300	0.45444000
C	0.74096200	8.35796700	-0.87046900	N	4.42813300	7.78858200	-3.95047800
C	1.18220400	9.44754400	-0.00418800	N	4.52987800	8.86945600	-3.57498700
C	0.77441100	9.14343500	1.28836100	N	4.26457700	6.60619600	-3.44282600
C	1.66717600	9.37730100	2.41787700	C	3.75929400	5.54488100	-4.31628900
C	1.46112200	8.61625000	3.57061800	H	4.30153900	5.57502700	-5.26086200
C	2.52628200	8.30816600	4.47969700	H	3.96312800	4.60288200	-3.80737400
C	2.21479700	7.07932300	5.13039900	H	2.68266400	5.65559800	-4.47538600
C	3.21530600	6.23267800	5.62899100				

Gas phase Absolute energy = -2717.82915989 a.u. Zero-point corrected energy = -2717.362146 a.u.

TS---f2---54–12

C	7.17505900	7.17505900	1.80863200	C	5.32950600	5.32950600	0.67271300
C	6.28733600	6.28733600	2.63337400	C	5.07378800	5.07378800	-0.79366900
C	4.87501600	4.87501600	2.60446700	C	3.82076200	3.82076200	-1.29193500
C	4.14210900	4.14210900	2.98615600	C	3.82006000	3.82006000	-2.51437300
C	2.81404100	2.81404100	2.52884900	C	2.75757400	2.75757400	-2.82731400
C	2.34504300	2.34504300	2.45528100	C	1.69968400	1.69968400	-1.91872900
C	1.32427500	1.32427500	1.56073600	C	1.05068000	1.05068000	-1.97646900
C	1.53009300	1.53009300	1.22929900	C	1.74566000	1.74566000	-0.65216700
C	1.10369600	1.10369600	0.01958400	C	2.76662200	2.76662200	-0.34975700
C	1.99010100	1.99010100	-0.73495000	C	6.37514700	6.37514700	2.80681200
C	1.98321600	1.98321600	-2.12458600	C	5.08122600	5.08122600	3.11198600
C	3.32783300	3.32783300	-2.65996400	C	4.67227600	4.67227600	2.77687900
C	3.73062500	3.73062500	-3.36918400	C	3.28596900	3.28596900	2.57757100
C	5.09379800	5.09379800	-3.35598600	C	2.82679400	2.82679400	1.75709300
C	5.59906800	5.59906800	-3.56743900	C	3.75752200	3.75752200	0.93276900
C	6.83011900	6.83011900	-2.82481100	C	3.29590000	3.29590000	-0.36894200
C	7.24007000	7.24007000	-2.33867600	C	4.16986500	4.16986500	-1.59789300
C	8.10419300	8.10419300	-1.19267000	C	5.49512800	5.49512800	-1.41085500
C	8.16503500	8.16503500	-0.30138700	C	5.98617300	5.98617300	-2.38814800
C	8.17073300	8.17073300	1.08881600	C	7.03919300	7.03919300	-2.07405700
C	6.67952800	6.67952800	0.88799300	C	7.60949000	7.60949000	-0.77862500
C	7.29073800	7.29073800	-0.41868600	C	8.17812300	8.17812300	-0.37344700
C	6.27934200	6.27934200	-1.43869700	C	8.10957200	8.10957200	1.04985500
C	6.29148500	6.29148500	-2.46707100	C	7.25389500	7.25389500	1.97030400
C	5.04555300	5.04555300	-3.07115000	C	6.82310200	6.82310200	1.58374100
C	4.72574900	4.72574900	-3.69505200	C	5.59311800	5.59311800	2.05194400
C	3.31233300	3.31233300	-3.58201100	C	5.11941200	5.11941200	1.08007200
C	2.78557900	2.78557900	-3.49022100	C	6.02075000	6.02075000	-0.08019600
C	1.51167100	1.51167100	-2.83547100	C	7.04881300	7.04881300	0.22844600
C	1.10118300	1.10118300	-2.24461900	N	4.05612900	4.05612900	-3.39604800
C	0.49223400	0.49223400	-0.93975500	N	3.45353700	3.45353700	-4.11972900
C	0.51674700	0.51674700	-0.74704900	N	4.46281400	4.46281400	-2.20362500
C	0.86847600	0.86847600	0.54812300	C	5.81223300	5.81223300	-1.98569700
C	1.38422000	1.38422000	0.57586100	H	5.84995200	5.84995200	-2.23938500
C	2.26800300	2.26800300	1.60552700	H	6.00898400	6.00898400	-0.91933600
C	3.08441300	3.08441300	1.07891200	H	6.56580100	6.56580100	-2.55524800
C	4.36308400	4.36308400	1.58011600				

Gas phase Absolute energy = -2717.84963396 a.u. Zero-point corrected energy = -2717.381543 a.u.

TS---g---11–10

C	1.61605000	1.12573600	2.07403000	C	-0.14681800	2.73188400	1.49190700
C	2.27873000	2.08953000	2.80541700	C	-0.54284600	3.08560600	0.09985900
C	1.66064600	3.38420500	3.03195900	C	-0.54512200	4.42952400	-0.32422400
C	2.69669300	4.33942400	3.19932700	C	-0.18592400	4.67051900	-1.67924500
C	2.51506000	5.70522700	2.86391500	C	0.38277700	5.92673100	-2.07829700
C	3.66736500	6.47178800	2.50907100	C	0.60484900	6.95457500	-1.12911600
C	3.58043900	7.60280100	1.67425800	C	1.64002100	7.87177400	-1.40869200
C	4.84831100	7.74074100	0.97912600	C	0.30302900	6.67345100	0.24848300
C	4.90056800	8.32921800	-0.26481700	C	-0.25706200	5.45168400	0.63897200
C	5.76130900	7.77817700	-1.30507800	C	3.69791600	2.31737100	2.60324900
C	5.01073600	7.84194800	-2.61736400	C	3.96421100	3.67224000	2.91952000
C	4.94107000	6.40873500	-3.07782900	C	5.04388200	4.38629900	2.32283400
C	3.75136400	5.82803300	-3.59017100	C	4.93981300	5.80486200	2.24102400
C	3.75918200	4.41737900	-3.64255100	C	5.61833500	6.54012400	1.24491500
C	2.54062400	3.62800200	-3.61188100	C	6.27274700	5.85093400	0.16491100
C	2.81073800	2.34457600	-3.00596700	C	6.22686600	6.48090000	-1.13834600
C	1.83598300	1.63611000	-2.26992500	C	5.85441300	5.66307300	-2.31385800
C	2.35143300	0.73592800	-1.28522200	C	5.75814900	4.25552300	-2.21505400
C	1.54138900	0.36681900	-0.15664800	C	4.76743600	3.63536000	-3.00433800
C	2.35603600	0.39093200	1.06243700	C	4.18208000	2.37034200	-2.60070800
C	0.33079800	1.43892600	1.49674800	C	4.60238000	1.72916800	-1.41141700
C	0.35534400	0.99023300	0.09426300	C	3.67421300	0.87482200	-0.78759900
C	-0.12441300	2.03743500	-0.75869600	C	3.63099400	0.75670900	0.69564700
C	0.55033000	2.31677700	-1.99710300	C	4.38443700	1.69803600	1.50200200
C	0.38483900	3.62619500	-2.48207300	C	5.40602300	2.42461300	0.86999000
C	1.35691200	4.26246800	-3.35065200	C	5.80396900	3.71523700	1.32713900
C	1.32680100	5.69880500	-3.15044100	C	6.32202700	4.45022600	0.21078800
C	2.45312300	6.50564900	-3.32626100	C	6.13509400	3.62908000	-0.97685600
C	2.48927900	7.72395800	-2.55705600	C	5.56558000	2.41552200	-0.58196200
C	3.70176100	8.37739500	-2.25726100	N	6.67542400	9.45875800	-3.16309600
C	3.68261400	8.77803400	-0.88472200	N	7.28842300	9.65499600	-2.22596700
C	2.43559200	8.45522000	-0.33665900	N	5.80069200	8.69608000	-3.71476000
C	2.33882400	7.91105100	0.99163800	C	5.04328100	9.20200700	-4.86241000
C	1.22489100	7.11403500	1.29110000	H	5.73196000	9.63417600	-5.58791200
C	1.27174600	6.08421100	2.28219700	H	4.54971700	8.33287200	-5.29949800
C	0.31557000	5.08540200	1.93327200	H	4.29188300	9.92911100	-4.54313900
C	0.46211200	3.74460000	2.32995600				

Gas phase Absolute energy = -2717.85216314 a.u. Zero-point corrected energy = -2717.384459 a.u.

Adduct---d---22–19

C	1.29023200	2.27803700	2.85577900	C	-0.87393500	3.36973900	2.66521200
C	1.85772600	3.44905300	3.34183000	C	-1.65879100	3.45277000	1.39943100
C	1.02473900	4.59215700	3.64690500	C	-2.10326100	4.69981800	0.89363000
C	1.80897100	5.75937500	3.48469200	C	-2.15873200	4.82602400	-0.50487000
C	1.23035400	7.00051100	3.11242000	C	-2.01268600	6.11989600	-1.13102000
C	2.04668000	7.94480400	2.42825500	C	-1.82670900	7.28345300	-0.34836100
C	1.49447600	8.91358700	1.56660000	C	-1.14351700	8.35424100	-0.95729800
C	2.49785600	9.23684700	0.56462700	C	-1.71496000	7.12567500	1.08194000
C	2.11364100	9.67010900	-0.68174000	C	-1.84657600	5.87903600	1.67803000
C	2.77035100	9.12901900	-1.85997100	C	3.09520700	3.94909400	2.78414400
C	1.71507800	8.77928700	-2.81652700	C	3.10863700	5.35546000	2.94315600
C	1.93126800	7.44859000	-3.31173700	C	3.80532500	6.20144900	2.04081400
C	0.82467400	6.54928200	-3.45204100	C	3.34940700	7.54098700	1.88650400
C	1.15644200	5.18186900	-3.41193600	C	3.57370700	8.26756400	0.70022500
C	0.21490800	4.16560800	-2.98907400	C	4.10703700	7.60695800	-0.46880800
C	0.92736900	3.06215600	-2.38302600	C	3.60372000	8.03944300	-1.76211800
C	0.36336000	2.25662200	-1.37643800	C	3.15990900	7.01691000	-2.75000400
C	1.29921300	1.64552500	-0.49244200	C	3.42822800	5.65084500	-2.53708900
C	0.90970700	1.00712100	0.81434800	C	2.45217100	4.73293700	-2.99168800
C	1.93285800	1.59803600	1.76825700	C	2.31462300	3.43616500	-2.36948200
C	-0.13198000	2.21884800	2.63988200	C	3.13884700	3.06993900	-1.29150700
C	-0.45362600	1.42248700	1.37199400	C	2.60534800	2.12704100	-0.37872400
C	-1.21095800	2.43851400	0.55505400	C	2.94766200	2.19081900	1.06907400
C	-0.96015900	2.67116900	-0.82686100	C	3.62684400	3.35961200	1.58726500
C	-1.55208900	3.83421900	-1.35103200	C	4.25653300	4.20283100	0.66335900
C	-1.00217200	4.54445000	-2.48392500	C	4.43797300	5.58989400	0.91760500
C	-1.32455300	5.95253800	-2.37927500	C	4.48922200	6.27122000	-0.33918900
C	-0.49154200	6.95825500	-2.90391400	C	4.22651700	5.27975500	-1.39354500
C	-0.59503600	8.23401400	-2.25940100	C	4.08202400	4.03729600	-0.79225700
C	0.50488500	9.15558600	-2.31272300	N	-0.23045900	-0.87585800	1.21564600
C	0.69767300	9.77189500	-0.99651600	N	0.86994000	-0.48854000	0.79687000
C	-0.25034700	9.23688000	-0.15646700	N	-1.11415000	0.12508200	1.45739400
C	0.09812200	8.85196900	1.20132300	C	-2.17850300	-0.12346700	2.40666100
C	-0.69028100	7.88068400	1.81931100	H	-2.99641200	0.57334200	2.20758200
C	-0.16874600	7.01964800	2.83564800	H	-2.53213700	-1.14401100	2.25805400
C	-0.90844900	5.80490700	2.81288000	H	-1.84189600	0.00430500	3.44336100
C	-0.35274900	4.59296600	3.24357100				

Gas phase Absolute energy = -2717.93450990 a.u. Zero-point corrected energy = -2717.462608 a.u.

Adduct---e1---9–10

C	3.94015200	2.56514900	2.84096900	C	1.76847700	3.66081600	2.49851500
C	4.52917700	3.80143300	3.09250700	C	0.93063700	3.55281000	1.26787700
C	3.69766100	4.98735900	3.19926600	C	0.49744700	4.70324500	0.58799400
C	4.49513200	6.13456400	2.80998500	C	0.39456100	4.61222200	-0.82018800
C	3.90352300	7.31981200	2.27322300	C	0.50806600	5.80735100	-1.65011000
C	4.68425300	8.13166000	1.43466200	C	0.70338500	7.08502400	-1.06503800
C	4.08644300	8.98099900	0.42140000	C	1.34008700	8.05569000	-1.85450600
C	5.00296200	9.12412000	-0.61400100	C	0.87973000	7.14321100	0.36497600
C	4.65021900	9.65773400	-1.96721900	C	0.79016500	6.00137500	1.15541100
C	5.29779000	8.83811900	-3.13154700	C	5.72602200	4.19371500	2.40275900
C	4.11527500	8.20624900	-3.85087300	C	5.72050700	5.65208100	2.30343700
C	4.32134000	6.82686800	-4.09868800	C	6.40318400	6.36044000	1.26264400
C	3.24757600	5.91431800	-4.06729900	C	5.93778200	7.66942800	0.92749800
C	3.60773500	4.55099100	-3.80557600	C	6.10687700	8.23106700	-0.37504600
C	2.67219300	3.59329300	-3.23921600	C	6.60495100	7.39349500	-1.43450800
C	3.40450200	2.58466400	-2.49234500	C	6.05354600	7.59146400	-2.73438900
C	2.86046800	1.93349800	-1.35865400	C	5.59830000	6.48955000	-3.47687000
C	3.81324500	1.43113300	-0.42391800	C	5.88030100	5.14750800	-3.07029300
C	3.44190000	1.23048600	0.95239400	C	4.88959500	4.16750900	-3.36750500
C	4.52155100	1.73996700	1.82249700	C	4.77137000	2.96058100	-2.55266000
C	2.51400000	2.51073400	2.62977800	C	5.63126800	2.74202400	-1.44826600
C	2.25757500	1.69170600	1.42746300	C	5.14754400	1.93166300	-0.40767100
C	1.33517200	2.38713600	0.56442800	C	5.53296700	2.20698300	1.00151400
C	1.56370700	2.42845400	-0.84312300	C	6.21198200	3.43555700	1.31747700
C	0.95143400	3.50991700	-1.51997100	C	6.81514000	4.14919900	0.22536900
C	1.47808100	4.04813800	-2.76276200	C	6.99391800	5.58269600	0.24614600
C	1.14086900	5.46265800	-2.86977800	C	7.02056100	6.07540400	-1.10727700
C	1.94247600	6.38815500	-3.57768900	C	6.70370400	4.96926100	-1.94518500
C	1.83697400	7.74500400	-3.15046300	C	6.56799200	3.78881400	-1.10925900
C	2.92091000	8.65736400	-3.37936000	N	5.91979400	10.96108900	-3.41363500
C	3.15209400	9.45867700	-2.19304100	N	6.06197700	9.83249600	-3.92495700
C	2.25068100	9.05465700	-1.24478200	N	5.23148800	10.96382500	-2.25966600
C	2.65499100	8.87034000	0.14512200	C	4.68323900	12.19846300	-1.74985100
C	1.91010100	8.01615000	0.93552400	H	5.32893600	13.01383500	-2.07673400
C	2.48319700	7.30303600	2.06067400	H	3.66142800	12.36934000	-2.11151900
C	1.76887800	6.11251300	2.23427000	H	4.67490400	12.15738600	-0.65732000
C	2.33666800	4.94428200	2.85127500				

Gas phase Absolute energy = -2717.90663303 a.u. Zero-point corrected energy = -2717.436302 a.u.

Adduct---e2---10–53

C	4.11079500	1.94830000	2.78439500	C	1.87976400	2.98095500	2.60860500
C	4.67342100	3.16647000	3.08424300	C	1.00292300	2.90759000	1.40656900
C	3.82701100	4.32957600	3.30668700	C	0.50946500	4.08168200	0.80289400
C	4.57011900	5.47643500	2.95493500	C	0.36206000	4.06170800	-0.60492000
C	3.93735200	6.66255100	2.49080300	C	0.42395800	5.28575500	-1.37115300
C	4.67695800	7.52712800	1.63770900	C	0.63951800	6.52724300	-0.73425600
C	4.04042200	8.38508900	0.72015500	C	1.25338500	7.54694200	-1.50088300
C	4.95140300	8.59901300	-0.38905900	C	0.85441900	6.52334500	0.69217400
C	4.48125900	8.93261900	-1.61975300	C	0.79216600	5.34568100	1.43193700
C	5.17563800	8.46113800	-2.89276000	C	5.85650200	3.62093900	2.37076300
C	3.97188000	7.82235600	-3.59328900	C	5.84378500	5.03358900	2.37333100
C	4.19542900	6.44456000	-3.88540700	C	6.45522300	5.78180400	1.33680500
C	3.09345200	5.51015300	-3.88302900	C	5.94758100	7.08551100	1.05340900
C	3.45419100	4.16407400	-3.74765000	C	6.07868100	7.66984900	-0.21591800
C	2.56445500	3.18158900	-3.17275300	C	6.56016600	6.90681700	-1.31876700
C	3.34329800	2.15729900	-2.50261100	C	6.17815800	7.27486200	-2.74983800
C	2.86313600	1.45992700	-1.38027400	C	5.46293800	6.08630800	-3.41281000
C	3.87631000	0.94407300	-0.50629600	C	5.77175100	4.75031000	-3.08809500
C	3.57307700	0.69056200	0.87597200	C	4.78461500	3.78231100	-3.36587900
C	4.68484400	1.15025900	1.71782100	C	4.71829300	2.55119400	-2.61238200
C	2.66654800	1.85258900	2.64668800	C	5.63539000	2.30263400	-1.56660500
C	2.39338800	1.09707400	1.42156500	C	5.19822600	1.45201800	-0.53196600
C	1.41228000	1.79505500	0.63107600	C	5.63886400	1.67319600	0.87584000
C	1.57807200	1.90456300	-0.78649100	C	6.32549000	2.90519800	1.21329600
C	0.92090000	2.99698900	-1.38554600	C	6.86561600	3.65507600	0.15984500
C	1.37753400	3.59259400	-2.62382500	C	7.02002300	5.06608600	0.24930300
C	1.03048400	4.99684400	-2.64060600	C	6.98624500	5.61397900	-1.07530100
C	1.80716500	5.95378100	-3.31822900	C	6.67503700	4.50255400	-1.99049300
C	1.71950900	7.29295300	-2.81586400	C	6.59951400	3.33233900	-1.25063300
C	2.78722100	8.22098700	-3.06008300	N	7.16982300	8.84737200	-4.00431100
C	3.05962800	8.95846500	-1.82657500	N	7.36494100	7.71183900	-3.54596300
C	2.16277000	8.52418100	-0.86721600	N	6.00842600	9.41913800	-3.58692000
C	2.62245900	8.28197800	0.48235000	C	5.45757600	10.50018200	-4.37426400
C	1.90535800	7.37080800	1.26622400	H	6.29047600	11.07838700	-4.77540200
C	2.52259000	6.63452100	2.32131300	H	4.83393500	10.13442600	-5.20025800
C	1.80552300	5.41400700	2.49326500	H	4.85358400	11.14109500	-3.72687800
C	2.41685900	4.26730800	3.01207400				

Gas phase Absolute energy = -2717.94022317 a.u. Zero-point corrected energy = -2717.468313 a.u.

Adduct---e3---11–12

C	7.20820000	-0.21127300	6.15812800	C	5.32108300	-1.18633600	4.92401500
C	6.43873100	0.88952000	6.48260400	C	5.35377800	-1.57741400	3.48356100
C	5.02156000	0.91090800	6.16340300	C	4.39477900	-1.07320400	2.57279200
C	4.62555500	2.26850900	5.99547900	C	4.83638800	-0.86130800	1.23444700
C	3.55049300	2.63186100	5.15357700	C	4.22174400	0.12185300	0.41709900
C	3.56243600	3.93749400	4.56757700	C	3.13227100	0.90435700	0.90523700
C	2.90806300	4.21121300	3.34013600	C	2.94425300	2.16857900	0.32915400
C	3.61758800	5.30168400	2.68607000	C	2.72290100	0.70556600	2.26958500
C	3.59210100	5.40337900	1.29291800	C	3.34001800	-0.26166700	3.07961400
C	4.80634700	5.67176700	0.59860800	C	6.94776300	2.22999800	6.26144900
C	4.89525700	5.03510300	-0.78222300	C	5.83102800	3.08685600	6.04074700
C	6.30645400	4.38232900	-0.78890000	C	5.93615100	4.26318700	5.25813800
C	6.34415000	2.85314500	-0.81556500	C	4.75980500	4.74218800	4.61322200
C	7.51841900	2.27756600	-0.35591700	C	4.82037800	5.53290300	3.42011700
C	7.60720400	0.88342200	-0.04755100	C	6.06651800	5.66127400	2.72820900
C	8.55474600	0.68375300	1.02341200	C	6.02393900	5.65095500	1.27378900
C	8.43557000	-0.36551100	1.93311000	C	6.94626100	4.88611000	0.50947800
C	9.04128700	-0.13813100	3.22814200	C	8.02081500	4.24044100	1.13040900
C	8.59502400	-0.88512000	4.38314600	C	8.39489600	2.96930000	0.60719500
C	8.50242200	0.00921300	5.53988100	C	9.01087900	2.00499700	1.43289800
C	6.59133100	-1.30941700	5.44861300	C	9.26357000	2.27621600	2.81376900
C	7.47287600	-1.64781200	4.32497700	C	9.32969500	1.15291000	3.68705600
C	6.70020200	-1.74250500	3.10868800	C	8.88654800	1.26051100	5.10919400
C	7.21474000	-1.20693100	1.87446500	C	8.15383000	2.43581500	5.52104100
C	6.24805400	-0.89875100	0.91273800	C	8.23560300	3.57584100	4.69039800
C	6.46929200	0.10270800	-0.10660600	C	7.19246500	4.52291500	4.62537500
C	5.22622300	0.70723500	-0.46135900	C	7.22203900	5.14737200	3.32228500
C	5.14631200	2.05014300	-0.87012800	C	8.22190700	4.47598200	2.53728800
C	3.86800200	2.71202100	-0.65563700	C	8.85042500	3.51655200	3.35639600
C	3.75437900	4.08424700	-0.62718300	N	6.17350100	5.71217500	-2.58869800
C	2.90183100	4.43367100	0.50530100	N	6.95677100	4.93000500	-2.02254700
C	2.41681800	3.27184500	1.10442400	N	5.01011500	5.91474600	-1.93046900
C	2.35033100	3.14810300	2.54752200	C	3.86326600	6.38176800	-2.67972100
C	2.40062600	1.85359700	3.09468600	H	4.23132600	7.00996600	-3.49122500
C	2.90707200	1.59649800	4.41342800	H	3.28017800	5.54930400	-3.09202200
C	3.43061700	0.27621700	4.43852400	H	3.22252600	6.97750700	-2.02485400
C	4.45325500	-0.10554000	5.33379200				

Gas phase Absolute energy = -2717.89985715 a.u. Zero-point corrected energy = -2717.430148 a.u.

Adduct---f1---54–53

C	5.31429500	4.24099800	5.16539100	C	2.97516500	4.83096800	5.62266200
C	5.63503200	5.57319000	4.98579300	C	1.80341500	4.30576600	4.87545000
C	4.64999100	6.60646000	5.26670200	C	0.86244500	5.17811100	4.30160400
C	4.93741000	7.72161000	4.44165500	C	0.27043000	4.76213100	3.07247200
C	3.91588800	8.61940200	4.02080200	C	-0.23650600	5.70866200	2.14096900
C	4.09269600	9.31093800	2.80130600	C	-0.12817500	7.09728900	2.38306400
C	2.99758500	9.78275600	2.03178600	C	-0.07267500	7.96464400	1.26341700
C	3.41158200	9.79179400	0.66508400	C	0.53804600	7.51198700	3.58962800
C	2.48338900	9.68131800	-0.36238300	C	1.01468400	6.58474200	4.52014500
C	2.83095400	8.82387500	-1.44602100	C	6.37390400	5.99005300	3.81570400
C	1.70804200	8.02195000	-1.71231200	C	6.01221000	7.33836200	3.53452300
C	2.13783800	6.70011800	-1.81179500	C	6.05394600	7.85886800	2.22019900
C	1.40525900	5.66628300	-1.18355600	C	5.17548500	8.92941800	1.89064100
C	2.11480900	4.47005700	-0.93622500	C	4.73524500	9.14458000	0.57552100
C	1.72390500	3.56984900	0.08282600	C	5.02117600	8.20543800	-0.44711600
C	2.88977400	2.89429800	0.60796600	C	4.14278700	8.12116400	-1.68712300
C	2.97505800	2.46396300	1.94041000	C	3.65968100	6.66173600	-2.08587100
C	4.30568700	2.34862100	2.47087300	C	4.33255000	5.52162800	-1.34576100
C	4.52014500	2.43861500	3.88214100	C	3.58051800	4.38777800	-1.04883700
C	5.69416600	3.28509600	4.15129700	C	4.03286800	3.43778100	-0.08394000
C	3.97703000	3.88852000	5.59707400	C	5.26576200	3.62437700	0.59055800
C	3.51172500	2.79816600	4.72734700	C	5.39229600	3.03526500	1.86573100
C	2.19815900	3.09316400	4.23854700	C	6.18522600	3.69787800	2.93175400
C	1.87864900	2.85873300	2.86524400	C	6.61737800	5.06925700	2.74078000
C	0.81817600	3.63189200	2.35149100	C	6.58855900	5.57388200	1.43057700
C	0.70512900	3.94587100	0.95727000	C	6.39409700	6.96648400	1.16344700
C	0.02363700	5.19510500	0.79872700	C	5.82571000	7.12084700	-0.13532700
C	0.29091100	6.04714000	-0.27634500	C	5.52125300	5.76127800	-0.62849100
C	-0.00153000	7.44552100	-0.08225700	C	5.97976300	4.84036600	0.33423300
C	0.60643900	8.42419300	-0.89023500	N	4.71190400	7.80123400	-3.82654300
C	1.08679000	9.46740500	-0.04620300	N	4.84139700	8.62002900	-2.90005100
C	0.70868500	9.17875900	1.28659800	N	3.97872300	6.70828000	-3.50816800
C	1.63573600	9.39192700	2.36343300	C	4.12102100	5.52645700	-4.33214700
C	1.47434200	8.63407900	3.53523000	H	4.31374500	5.85962300	-5.35217300
C	2.56697900	8.32007600	4.39694900	H	4.94273000	4.88376300	-3.99388200
C	2.27132000	7.10133800	5.07325100	H	3.18786000	4.95746300	-4.30984500
C	3.28586400	6.25123300	5.53481400				

Gas phase Absolute energy = -2717.87704485 a.u. Zero-point corrected energy = -2717.407546 a.u.

Adduct---f2---54–12

C	7.14678100	2.08967300	1.64791500	C	5.28844300	0.96054800	0.50218500
C	6.26740500	2.75509700	2.47460800	C	5.03738600	1.00819700	-0.96248300
C	4.84926700	2.43539100	2.43717800	C	3.79093300	1.42782900	-1.46478100
C	4.13487600	3.59071700	2.81870100	C	3.80263400	2.14502800	-2.68859600
C	2.81058700	3.83641900	2.35527400	C	2.75606000	3.07587500	-3.00455900
C	2.36502000	5.18030400	2.28143500	C	1.70592600	3.31540800	-2.09784800
C	1.35277900	5.58157300	1.38162300	C	1.07742400	4.58866200	-2.15793300
C	1.59423200	6.97306500	1.04549300	C	1.73533400	2.63168700	-0.83289200
C	1.17889100	7.47530000	-0.16098800	C	2.73970000	1.71745300	-0.52648400
C	2.10460600	8.30504000	-0.92035200	C	6.38034200	4.19024400	2.65129800
C	2.05273800	7.88241700	-2.30766100	C	5.09127300	4.68988500	2.95228600
C	3.39752800	7.95295200	-2.97352100	C	4.70845500	6.01529100	2.61704000
C	3.79377000	6.58678600	-3.52529000	C	3.32806500	6.28221700	2.40783100
C	5.13675500	6.28900500	-3.49065200	C	2.89630700	7.33753900	1.58240100
C	5.62711700	4.95481300	-3.70245200	C	3.84137700	8.05016100	0.76406200
C	6.85048200	4.75251300	-2.96281700	C	3.40083800	8.48866000	-0.54078700
C	7.24474900	3.48967300	-2.48717100	C	4.31189700	8.53138400	-1.78522600
C	8.11343100	3.50815500	-1.34143800	C	5.60759600	7.79321900	-1.55133700
C	8.15063800	2.38004200	-0.45660600	C	6.06975900	6.91904000	-2.52165200
C	8.15954700	2.84383500	0.93807300	C	7.08543600	5.95742800	-2.21076700
C	6.63963100	1.09191400	0.72458500	C	7.66222700	5.89449800	-0.91574200
C	7.25910400	1.35698400	-0.58035900	C	8.20447200	4.65433000	-0.51574100
C	6.25151200	1.36824400	-1.60263000	C	8.12430600	4.21953900	0.90475100
C	6.28059400	2.37183600	-2.62473700	C	7.27841400	4.95853700	1.82518800
C	5.04039700	2.63919700	-3.23484700	C	6.87318100	6.24070300	1.43971500
C	4.74035100	3.90956200	-3.84855300	C	5.64682300	6.81650700	1.89831900
C	3.33661800	4.17362400	-3.74858700	C	5.19853300	7.75822800	0.93092700
C	2.83948900	5.48196500	-3.64583400	C	6.10696700	7.66679900	-0.22718600
C	1.55348900	5.60362200	-3.01026800	C	7.11508100	6.74977100	0.08929000
C	1.16296800	6.86546300	-2.42624200	N	4.08947600	9.99749600	-3.59078800
C	0.55548800	6.59806000	-1.12138100	N	3.47018900	9.01097400	-4.02332100
C	0.54933400	5.23144900	-0.92857300	N	4.50641700	9.88393700	-2.31383700
C	0.88609200	4.67369300	0.36480600	C	5.57570500	10.75143900	-1.86539200
C	1.38362300	3.36211700	0.39505600	H	5.45018200	11.71455100	-2.36061100
C	2.25253800	2.90976900	1.42548800	H	5.49146300	10.88905700	-0.78399900
C	3.05507500	1.84660300	0.90258700	H	6.56623500	10.34320600	-2.09954900
C	4.32545900	1.56894500	1.40862900				

Gas phase Absolute energy = -2717.91483218 a.u. Zero-point corrected energy = -2717.442893 a.u.

Adduct---g---11–10

C	1.79248300	1.20641100	1.98125900	C	0.01980900	2.79681200	1.40239200
C	2.46549500	2.20279200	2.69089300	C	-0.41087400	3.13243500	0.02182000
C	1.84266200	3.49007500	2.88553300	C	-0.42381300	4.46493500	-0.40785000
C	2.89231500	4.48777500	2.99555900	C	-0.08254500	4.70423100	-1.77122500
C	2.66931400	5.86353700	2.64959800	C	0.47856200	5.97819300	-2.18207600
C	3.80270400	6.64692900	2.26630700	C	0.67116200	7.04589600	-1.25189300
C	3.68225600	7.76546800	1.43331800	C	1.65994200	7.99917500	-1.57166800
C	4.94454500	7.91970100	0.72097800	C	0.41637400	6.76147200	0.12033800
C	4.96156500	8.49730000	-0.51117000	C	-0.11757600	5.49891800	0.54376400
C	5.93876000	8.06001700	-1.59256500	C	3.86248200	2.44714500	2.44910400
C	5.08638900	8.02493100	-2.89237200	C	4.11821700	3.85569200	2.71408900
C	4.98997600	6.56302700	-3.25530700	C	5.20480100	4.57008000	2.09561600
C	3.82428800	5.95353600	-3.71515300	C	5.09183700	6.00091600	1.98981200
C	3.84066900	4.52347500	-3.74336200	C	5.76035400	6.73390500	1.00902900
C	2.62466900	3.70867600	-3.70661900	C	6.42790200	6.04166600	-0.07774600
C	2.91627600	2.42322400	-3.11033100	C	6.33894000	6.61928300	-1.36475300
C	1.94701500	1.69305700	-2.36185000	C	5.93425800	5.82605700	-2.46733800
C	2.48099800	0.79947200	-1.38692800	C	5.84849700	4.40329800	-2.35912000
C	1.68903300	0.42568000	-0.25269800	C	4.84440600	3.76253100	-3.13426200
C	2.51821700	0.49089800	0.96803500	C	4.27235500	2.47861100	-2.71586500
C	0.51093300	1.50738400	1.41178200	C	4.71505900	1.83949400	-1.52753200
C	0.49772300	1.03184400	0.00734900	C	3.81251000	0.97223200	-0.89562400
C	0.00875000	2.07291200	-0.84304100	C	3.79087100	0.86654400	0.58389800
C	0.66506400	2.35135300	-2.08221200	C	4.52816800	1.82871500	1.36778000
C	0.48399400	3.67726000	-2.56528500	C	5.55137600	2.57228800	0.69507100
C	1.44070700	4.32415300	-3.44538700	C	5.95574200	3.89525500	1.13165700
C	1.39043400	5.77093100	-3.25219500	C	6.47214500	4.62338400	-0.00296600
C	2.50367000	6.61405800	-3.44576000	C	6.24355100	3.81357100	-1.14299800
C	2.50371200	7.84639700	-2.73913200	C	5.66049600	2.55243900	-0.70256200
C	3.73424200	8.49270900	-2.44800000	N	6.91616000	9.43164000	-3.05054800
C	3.73128800	8.90205000	-1.11663400	N	7.03211800	9.01689900	-1.88329500
C	2.46436100	8.59000800	-0.52995500	N	5.91463600	8.84227300	-3.76412300
C	2.41658800	8.06344800	0.78372200	C	5.35625800	9.59349200	-4.86891800
C	1.31687100	7.23837700	1.12891500	H	6.17031700	10.13154700	-5.35537000
C	1.41230600	6.21668800	2.12626300	H	4.90988700	8.89516800	-5.58122600
C	0.46814500	5.17507300	1.79287600	H	4.59169300	10.30661700	-4.53534900
C	0.64628300	3.82172400	2.21053200				

Gas phase Absolute energy = -2717.91960710 a.u. Zero-point corrected energy = -2717.430148 a.u.

S9.2 Methyl azide additions to $Sc_2@C_{66}$

TS---d---22–19

C	1.36667100	-3.23535600	-1.18278800	C	0.97763300	0.26391100	-1.08395400
C	0.03667600	-3.55771300	-1.57842000	C	-0.10369600	1.19516400	-0.96611700
C	-0.78037800	-2.63277000	-2.34676500	C	-0.27793000	1.83405300	0.28853000
C	-2.14790700	-2.94075700	-2.08118000	C	-1.56537500	2.29195800	0.69590300
C	-3.18183600	-1.95995700	-2.16292000	C	-2.69436600	2.11742100	-0.14707000
C	-4.35843100	-2.16740000	-1.38959600	C	-3.97730900	2.01778000	0.48405300
C	-5.18015900	-1.08166100	-0.95467600	C	-2.53063500	1.43983500	-1.38504200
C	-5.83563100	-1.49251500	0.27714100	C	-1.23956400	0.98099900	-1.79261500
C	-6.28966900	-0.54535800	1.23384200	C	-0.85729000	-4.31193400	-0.71518900
C	-5.99316900	-0.82886100	2.63086800	C	-2.19592300	-3.97570000	-1.07836700
C	-5.41659200	0.35408000	3.24156000	C	-3.27623800	-4.03671800	-0.14902700
C	-4.21500800	-0.02908200	3.92198900	C	-4.40618400	-3.20395000	-0.38536700
C	-2.98462600	0.73384300	3.77540000	C	-5.25752700	-2.76592300	0.67538800
C	-1.78314000	0.04758300	4.08728500	C	-4.87137600	-2.99874900	2.04453200
C	-0.52583700	0.44133500	3.53623300	C	-5.18307300	-1.96866800	3.00601300
C	0.32667700	-0.69525200	3.42151300	C	-4.13830400	-1.48314400	3.87316800
C	1.32467400	-0.78916800	2.41090100	C	-2.89105900	-2.17607500	4.01053800
C	1.73384700	-2.12338900	2.03558700	C	-1.73541600	-1.39263600	4.26593500
C	2.42050600	-2.40682300	0.79044500	C	-0.44626700	-1.84534700	3.85382900
C	1.72743100	-3.54763800	0.18378000	C	-0.29848000	-3.08695500	3.18419600
C	1.82139300	-1.88049000	-1.44372500	C	0.82039300	-3.22663000	2.30055400
C	2.52308200	-1.33356100	-0.24748500	C	0.75217300	-4.05481300	1.12571300
C	1.82862600	-0.07106700	0.04939100	C	-0.53232500	-4.51739000	0.67420900
C	1.37060500	0.27168200	1.37434500	C	-1.59892600	-4.50151400	1.61090800
C	0.41725600	1.32430700	1.45739800	C	-2.96432700	-4.36436300	1.20350300
C	-0.48086100	1.44516800	2.55760000	C	-3.69921800	-3.76452800	2.27641600
C	-1.68980100	2.06968400	2.12585600	C	-2.75153600	-3.39955900	3.30127200
C	-2.93552900	1.79584700	2.74660200	C	-1.46000400	-3.85187600	2.88886400
C	-4.12055700	2.02647300	1.93376900	Sc	0.30720100	-1.85940400	0.18140600
C	-5.36893800	1.39131600	2.23816100	Sc	-4.11343100	-0.29763600	1.59003800
C	-5.91645300	0.84537000	1.01037300	N	4.86256000	-1.99533300	0.16260700
C	-5.03660100	1.21663800	-0.07770600	N	4.58128000	-2.79376500	0.94714800
C	-4.72094800	0.27386900	-1.12400200	N	4.28507000	-1.03851600	-0.46622400
C	-3.50563500	0.47388400	-1.82904200	C	4.68879400	-0.76667900	-1.84506800
C	-2.79214800	-0.61402100	-2.42848100	H	4.07196500	0.07054800	-2.17522600
C	-1.40464300	-0.26838200	-2.48887900	H	4.51567300	-1.62745400	-2.49939700
C	-0.38075800	-1.25338100	-2.48614500	H	5.73724600	-0.46694700	-1.87359300
C	0.90033900	-0.87713200	-1.95498200				

Gas phase Absolute energy = -2810.86531821 a.u. Zero-point corrected energy = -2810.394165 a.u.

Solvent phase Absolute energy = -2810.89704389 a.u.

TS---e1---9–10

C	-4.75163600	2.11492800	2.71854100	C	-5.30981200	0.54666700	-0.39824500
C	-3.60032600	2.86315400	2.34751900	C	-4.54223600	0.24227800	-1.57151800
C	-3.37175000	3.27941600	0.97199900	C	-4.12691300	-1.10439900	-1.74833700
C	-1.96410500	3.45183800	0.80324700	C	-2.94209500	-1.40199600	-2.48507300
C	-1.32535300	3.28969700	-0.46045300	C	-2.16395300	-0.36342100	-3.05925700
C	0.05223200	2.92597000	-0.46227000	C	-0.76272200	-0.61792500	-3.24028200
C	0.65336300	2.22520300	-1.55494400	C	-2.55645900	0.98512300	-2.85246600
C	1.76735300	1.46729400	-1.03151500	C	-3.73714300	1.28397400	-2.10246400
C	2.38308800	0.34314900	-1.73414900	C	-2.30073700	2.61290800	2.94919000
C	2.60505300	-0.86111200	-0.84103200	C	-1.30485900	3.04289000	2.01871300
C	1.90730600	-2.01058500	-1.41995100	C	-0.00275300	2.46633600	1.98034700
C	1.15322100	-2.66715300	-0.40053300	C	0.71008800	2.51841500	0.74841800
C	-0.20696300	-3.12019200	-0.62963700	C	1.72345600	1.56500300	0.40857600
C	-1.00203800	-3.33477800	0.52636000	C	1.91100600	0.40077900	1.24247500
C	-2.42708100	-3.27792300	0.47712100	C	2.24243500	-0.82856600	0.57417700
C	-2.93405600	-2.84650300	1.74194500	C	1.45623300	-2.00085200	0.85704900
C	-4.14553200	-2.11530800	1.84266400	C	0.56038800	-2.06163200	1.97421800
C	-4.28935500	-1.27580700	3.02107500	C	-0.60405700	-2.86151700	1.83716000
C	-5.21421700	-0.18180700	3.05131200	C	-1.78546500	-2.56393900	2.58339300
C	-4.53610100	0.97602400	3.60138300	C	-1.81287900	-1.45681800	3.47120700
C	-5.60146900	1.63852500	1.63551800	C	-3.08416400	-0.83939000	3.71213700
C	-5.87290900	0.22794300	1.83426900	C	-3.20147400	0.57014800	3.99155800
C	-5.59490100	-0.46377400	0.61095400	C	-2.06908400	1.42746400	3.73683300
C	-4.82011500	-1.69490900	0.59524600	C	-0.79675800	0.80710800	3.63292400
C	-4.22226100	-2.04245000	-0.64326200	C	0.26524600	1.37156500	2.85370300
C	-3.06484100	-2.87641300	-0.70388100	C	1.13011500	0.31302400	2.42816400
C	-2.28440200	-2.53136900	-1.84955500	C	0.52024200	-0.92920600	2.83088700
C	-0.87861600	-2.70432800	-1.87425300	C	-0.66367400	-0.62705700	3.57359600
C	-0.14337200	-1.85784400	-2.80168800	Sc	-3.69692000	0.51977700	1.60680900
C	1.25566000	-1.59557500	-2.63358500	Sc	0.36481000	-0.51355100	-0.93176300
C	1.48348100	-0.17653100	-2.81512700	N	4.79245500	-0.13125600	-1.99697200
C	0.21682100	0.43331000	-3.15678400	N	4.83471000	-1.03368700	-1.28656400
C	-0.18270900	1.70432400	-2.60604900	N	4.00630000	0.81541600	-2.33436900
C	-1.56955100	1.99511000	-2.55649400	C	4.04322900	1.32745400	-3.70219400
C	-2.12627300	2.85906300	-1.55781000	H	3.27122900	2.09776500	-3.74597000
C	-3.49116600	2.48334500	-1.33908400	H	3.82315700	0.54771600	-4.43814700
C	-4.15083200	2.72269200	-0.10609600	H	5.01282500	1.78532600	-3.90253900
C	-5.22954200	1.83169200	0.24838300				

Gas phase Absolute energy = -2810.87219958 a.u. Zero-point corrected energy = -2810.400956 a.u.

Solvent phase Absolute energy = -2810.90379343 a.u.

TS---e2---10–53

C	-4.41438100	-0.57091400	6.21045600	C	-2.07400000	-3.21382600	6.01545700
C	-5.09891900	-0.84207900	4.99299800	C	-1.51826500	-4.05491000	4.99590900
C	-5.16369900	-2.18233200	4.43348100	C	-0.19281900	-3.77701200	4.56937400
C	-5.36329200	-2.05027000	3.02311900	C	0.22914200	-4.11441600	3.24704000
C	-4.91430900	-3.03740100	2.09633700	C	-0.66812600	-4.73163600	2.33921600
C	-4.64252800	-2.62373500	0.76134200	C	-0.44943400	-4.50366400	0.93984100
C	-3.71421900	-3.32377100	-0.07243100	C	-2.00879800	-4.96795900	2.74772500
C	-3.15997200	-2.36828800	-1.01792300	C	-2.43186900	-4.62663400	4.06940200
C	-1.90621000	-2.56931300	-1.63722600	C	-5.08024400	0.09390500	3.88012500
C	-1.00667300	-1.39004500	-1.81910500	C	-5.31504900	-0.65285200	2.68410000
C	0.30197600	-1.79875800	-1.22677400	C	-4.81730000	-0.23408700	1.41408300
C	0.69265600	-0.85041800	-0.22157100	C	-4.59897300	-1.22465500	0.41998300
C	1.26594600	-1.27543200	1.05063800	C	-3.62992700	-1.04764100	-0.62282100
C	1.21175400	-0.33010600	2.10602600	C	-2.72106000	0.05520400	-0.57677200
C	1.24790000	-0.72495900	3.48069500	C	-1.37616700	-0.11730900	-1.11897600
C	0.53673600	0.22768500	4.27487900	C	-0.28210900	0.21108000	-0.20419300
C	-0.13329100	-0.15016900	5.46599600	C	-0.46514400	1.06099300	0.92941700
C	-1.23991500	0.70044600	5.87618800	C	0.40019400	0.86542000	2.03429500
C	-2.25748500	0.22622400	6.76741500	C	-0.01512600	1.20886600	3.35877600
C	-3.55067200	0.60224700	6.22916800	C	-1.30313600	1.75438800	3.58565000
C	-3.63409900	-1.66310100	6.77839300	C	-1.89851800	1.51928000	4.86853000
C	-2.30890800	-1.17488900	7.10717900	C	-3.32642600	1.39078700	5.03380400
C	-1.34342000	-2.07490000	6.55004000	C	-4.14382900	1.19109900	3.86173200
C	-0.18920900	-1.58811900	5.81154300	C	-3.58076400	1.55312300	2.61076000
C	0.42784700	-2.51663100	4.93629400	C	-3.97634000	0.91782200	1.39066500
C	1.18976000	-2.08333800	3.80625200	C	-2.89332400	1.00561600	0.46141900
C	1.11508200	-3.06509900	2.77052400	C	-1.76845200	1.58183300	1.15866100
C	1.22037200	-2.70988800	1.40137900	C	-2.18761700	1.91013100	2.47965400
C	0.60595800	-3.62548700	0.45256800	Sc	-2.64918100	-0.94075600	4.93573200
C	0.23862400	-3.20009700	-0.86463500	Sc	-1.16042500	-2.10991100	0.41643300
C	-1.10229900	-3.67254300	-1.13429000	N	-0.94140600	0.30977200	-3.61437200
C	-1.53772100	-4.46292000	-0.00156000	N	-1.18649400	1.18291300	-2.90182700
C	-2.88633000	-4.35633600	0.49260800	N	-0.93904800	-0.97179400	-3.58994900
C	-3.10796500	-4.71521500	1.84875200	C	0.10372500	-1.66993300	-4.34031300
C	-4.16774100	-4.13659400	2.61627100	H	-0.01054200	-1.47785900	-5.40819600
C	-3.79612700	-4.16523500	3.99920500	H	-0.05690400	-2.73296000	-4.15368900
C	-4.30944500	-3.22882300	4.93501700	H	1.10771000	-1.38978300	-4.00430300
C	-3.48528500	-2.92324900	6.07865900				

Gas phase Absolute energy = -2810.86588721 a.u. Zero-point corrected energy = -2810.394549 a.u.

Solvent phase Absolute energy = -2810.89778510 a.u.

TS---e3---11–12

C	-4.09099100	1.88418900	1.78158100	C	-4.15139100	-1.53994000	0.92437700
C	-3.44578200	2.36024400	0.60914400	C	-3.43796700	-2.40763600	0.03217600
C	-3.55560300	1.66413000	-0.66132800	C	-2.46975300	-3.27007900	0.60528700
C	-2.40934600	2.00996200	-1.44244100	C	-1.34753000	-3.72360800	-0.15987100
C	-1.87740200	1.12560700	-2.42650800	C	-1.18303600	-3.30407600	-1.50410800
C	-0.49360200	1.23602800	-2.74081800	C	0.15666400	-3.24952600	-2.01745500
C	0.26039500	0.13895700	-3.26351500	C	-2.12660900	-2.39882300	-2.06276900
C	1.64864500	0.33048700	-2.87896400	C	-3.25133900	-1.95436500	-1.30310200
C	2.55041700	-0.76135800	-2.76058700	C	-2.13086400	2.97662200	0.65726900
C	3.40719400	-0.78917100	-1.58641300	C	-1.53264400	2.81432500	-0.63052700
C	3.42103800	-2.15255700	-0.98958000	C	-0.11830100	2.74603400	-0.79776800
C	3.10682100	-1.97700000	0.44464500	C	0.38491200	2.04555000	-1.93377800
C	2.01141600	-2.72599500	1.07711800	C	1.68639500	1.45840900	-1.95547100
C	1.51462200	-2.20393500	2.29596300	C	2.44311800	1.37528600	-0.73289400
C	0.21870600	-2.55638100	2.77944700	C	3.23574500	0.18395600	-0.52422800
C	-0.31581700	-1.47810700	3.54772300	C	3.10166800	-0.52429600	0.70898200
C	-1.71190500	-1.25118400	3.64794500	C	2.44478700	0.04145100	1.84525700
C	-2.11721800	0.10947200	3.96317100	C	1.77908900	-0.84563300	2.73225700
C	-3.43337400	0.58613100	3.64750200	C	0.65484800	-0.39802500	3.48648900
C	-3.30777600	1.88198300	3.00827600	C	0.20030000	0.94334500	3.39402500
C	-4.72555800	0.57734800	1.69834000	C	-1.18548400	1.19085100	3.66506700
C	-4.31092200	-0.22291200	2.83518900	C	-1.90662600	2.24795300	3.00000800
C	-3.85939100	-1.49602300	2.35052400	C	-1.31788600	2.87906600	1.84353600
C	-2.61277300	-2.08365700	2.81758900	C	0.08365900	2.73561100	1.67066600
C	-2.03103700	-3.06174600	1.97201100	C	0.69109400	2.76730100	0.37343000
C	-0.63023600	-3.35298000	2.00240300	C	1.90003400	1.99889800	0.41875300
C	-0.20001500	-3.80216400	0.72033300	C	1.96372200	1.37123600	1.71421500
C	1.12439100	-3.55807200	0.26066300	C	0.84813600	1.82362100	2.48466500
C	1.31234800	-3.53417900	-1.18089400	Sc	-2.52659200	0.30500600	1.66558700
C	2.44304100	-2.91009900	-1.78524400	Sc	1.28573200	-1.17098900	-1.01566400
C	1.97900100	-2.09467700	-2.88821400	N	5.46733100	-2.96400300	0.18652900
C	0.55021900	-2.29066500	-3.01865300	N	5.01446800	-2.78473800	1.23238400
C	-0.32434300	-1.17698500	-3.28809600	N	5.10493000	-2.98020000	-1.03678800
C	-1.67944400	-1.30030800	-2.88434700	C	6.02809900	-2.43093600	-2.02882300
C	-2.48019000	-0.16118400	-2.55719800	H	6.92947300	-3.04383400	-2.08378100
C	-3.50643000	-0.57693100	-1.64806000	H	6.28808000	-1.38844600	-1.81602200
C	-4.08594700	0.32454900	-0.71755500	H	5.50610300	-2.48541200	-2.98529500
C	-4.60410500	-0.23600400	0.50713000				

Gas phase Absolute energy = -2810.86972220 a.u. Zero-point corrected energy = -2810.398186 a.u.

Solvent phase Absolute energy = -2810.90146095 a.u.

TS---f1---54–53

C	-2.42135400	2.61033900	3.56070300	C	-4.10943200	1.73603700	0.58412900
C	-1.14558800	2.85832100	2.98582300	C	-3.75037100	1.26763800	-0.72258700
C	-0.99882500	3.28812500	1.60551900	C	-3.97559300	-0.10354200	-1.00706300
C	0.30389000	2.89359500	1.16757300	C	-3.17734400	-0.78493000	-1.97464900
C	0.58955600	2.61362000	-0.20125000	C	-2.14350000	-0.10125200	-2.66753700
C	1.66620300	1.72547300	-0.48739800	C	-1.03283400	-0.88236300	-3.12739900
C	1.72832700	0.96214300	-1.69648700	C	-1.88378400	1.25874400	-2.34682900
C	2.49602100	-0.24211400	-1.42003600	C	-2.68455900	1.94070800	-1.37952700
C	2.32719300	-1.43623500	-2.17347100	C	0.01225500	2.04032600	3.31415900
C	2.23575900	-2.68381700	-1.43265000	C	0.92370200	2.12763900	2.21881700
C	1.07682500	-3.41609300	-1.88961000	C	1.83535300	1.07559600	1.90909200
C	0.30186600	-3.81732600	-0.76101800	C	2.27739700	0.95716900	0.56495600
C	-1.13054200	-3.63521900	-0.72601000	C	2.71193700	-0.29208800	0.01654500
C	-1.74675800	-3.64733600	0.55155900	C	2.52060100	-1.50326800	0.75526200
C	-2.99453600	-2.99826200	0.78397800	C	2.29858500	-2.75917200	0.03608400
C	-3.05030800	-2.52505700	2.13190600	C	1.13412900	-3.60786200	0.45097100
C	-3.81081600	-1.38313800	2.49197700	C	0.43544400	-3.28440400	1.69901800
C	-3.38617700	-0.68408300	3.69549000	C	-0.96019900	-3.50129000	1.76469100
C	-3.74477100	0.68391200	3.93021700	C	-1.76244400	-2.81533100	2.73079500
C	-2.55895700	1.40025600	4.35954800	C	-1.17531300	-1.90235300	3.64011100
C	-3.56354800	2.63709900	2.65897900	C	-2.00968200	-0.84901600	4.14162200
C	-4.36808100	1.44975700	2.87732900	C	-1.47357000	0.44743700	4.46870300
C	-4.61860900	0.83369500	1.60760700	C	-0.14699900	0.78807400	4.01101200
C	-4.44879300	-0.59791400	1.41321100	C	0.70867200	-0.28402400	3.64537000
C	-4.26502600	-1.02924100	0.07403200	C	1.75009800	-0.12257500	2.67629300
C	-3.60371800	-2.25514100	-0.23717100	C	2.00545300	-1.39135400	2.06471100
C	-2.96030100	-2.14055200	-1.50643000	C	1.01100300	-2.32245000	2.56164700
C	-1.77466800	-2.85881000	-1.80385500	C	0.21527400	-1.63475600	3.53016400
C	-0.92728600	-2.30274500	-2.84085500	Sc	-2.35064600	0.83704300	2.23084500
C	0.45741600	-2.65494600	-2.94318300	Sc	0.42778200	-1.46625000	-1.06861500
C	1.22811300	-1.44205300	-3.12960800	N	3.25998500	-4.95090900	0.86742100
C	0.29846700	-0.33512800	-3.21529100	N	3.90357600	-4.02261700	0.60619900
C	0.57900500	0.92058500	-2.56287800	N	2.05346500	-5.33278600	0.77715100
C	-0.53039900	1.74292800	-2.23007900	C	1.50854500	-6.14284200	1.86474700
C	-0.49465800	2.65548100	-1.12667500	H	1.95809100	-7.13829200	1.85453700
C	-1.83270000	2.85086100	-0.65420700	H	0.44063400	-6.23600400	1.66187000
C	-2.11103000	3.20904900	0.69124000	H	1.65090200	-5.67248800	2.84333800

Gas phase Absolute energy = -2810.86923735 a.u. Zero-point corrected energy = -2810.397381 a.u.

Solvent phase Absolute energy = -2810.90061175 a.u.

TS---f2---54–12

C	-2.93373700	-0.14587900	4.43428700	C	-4.06927100	-1.59122400	1.41476900
C	-2.23767400	0.95395200	3.86129300	C	-3.70434500	-1.55303400	0.02854800
C	-2.62302900	1.51859000	2.57675100	C	-3.02438100	-2.68148200	-0.49899300
C	-1.46710900	2.14715500	2.01882000	C	-2.13491700	-2.53718100	-1.60626100
C	-1.28281900	2.28787600	0.61238400	C	-1.92012700	-1.26760800	-2.20315800
C	0.05021500	2.39899200	0.12094500	C	-0.65904800	-1.04801700	-2.85037100
C	0.40397400	2.00450200	-1.20702100	C	-2.56573300	-0.12954400	-1.64546500
C	1.79759900	1.59031600	-1.18246100	C	-3.45205900	-0.27275100	-0.53446500
C	2.33029400	0.68238500	-2.13747200	C	-0.79581900	1.09446600	3.98603400
C	3.19479700	-0.37836100	-1.63711100	C	-0.34316100	1.88869700	2.88493300
C	2.77039700	-1.63909400	-2.20406600	C	0.96937700	1.76885200	2.34852700
C	2.70424700	-2.65066100	-1.15361000	C	1.17017500	2.13485500	0.98826600
C	1.44086800	-3.39635000	-0.99793000	C	2.22025100	1.56707200	0.20152100
C	1.18769300	-3.93438900	0.28209800	C	2.97591000	0.44988800	0.70488800
C	-0.12083300	-4.33404900	0.68616200	C	3.41520600	-0.54748600	-0.22422800
C	-0.25893500	-4.17730000	2.09930000	C	3.30163200	-1.98974400	0.07845300
C	-1.51251500	-3.88855200	2.69464100	C	2.75328100	-2.35197900	1.39338500
C	-1.47066700	-3.22400200	3.98838300	C	1.87562500	-3.45393900	1.47671500
C	-2.59456900	-2.48845600	4.48906600	C	0.98228300	-3.60166100	2.58463600
C	-2.12018500	-1.21585900	4.99808500	C	0.95240800	-2.63364000	3.61832000
C	-3.93505300	-0.79367700	3.59674700	C	-0.27564800	-2.47415100	4.34185900
C	-3.71846200	-2.22717300	3.62258100	C	-0.67633300	-1.19907500	4.88382300
C	-3.69799100	-2.70624100	2.27298500	C	0.01019000	-0.00877200	4.44232800
C	-2.66755800	-3.62184800	1.80593200	C	1.28709100	-0.18158300	3.84634500
C	-2.46371200	-3.66899500	0.40652100	C	1.80949800	0.74253200	2.88385100
C	-1.21221200	-4.08045700	-0.15221200	C	2.73793700	0.05227600	2.04867000
C	-1.00798300	-3.43057700	-1.40221000	C	2.67529800	-1.34855200	2.39218900
C	0.29661200	-3.13680100	-1.88166400	C	1.78298300	-1.48885400	3.49995500
C	0.39569700	-2.05621200	-2.84985300	Sc	-1.92291700	-1.23901500	2.79862700
C	1.63911600	-1.37771200	-3.06115800	Sc	1.12166800	-0.81457300	-1.01389200
C	1.38168700	0.04862800	-3.03687700	N	4.93379000	-3.74974700	-0.69425300
C	-0.04415400	0.25233300	-2.88057400	N	4.14787800	-4.16448100	-1.44114800
C	-0.54985000	1.29084300	-2.01526700	N	5.07703700	-2.70372800	0.01906000
C	-1.85978400	1.11868100	-1.49602000	C	5.74741900	-2.83216900	1.31126900
C	-2.25472900	1.68863400	-0.24252600	H	5.65273300	-1.85769600	1.79317900
C	-3.30146800	0.88600500	0.31281900	H	6.80651000	-3.05163200	1.16234200
C	-3.53644000	0.81627200	1.71062800	H	5.28489900	-3.59639800	1.94437600
C	-4.13233900	-0.39552400	2.21814700				

Gas phase Absolute energy = -2810.86390244 a.u. Zero-point corrected energy = -2810.392339 a.u.

Solvent phase Absolute energy = -2810.89562453 a.u.

TS---g---11–10

C	-6.39763100	1.41018200	2.56650100	C	-6.26977400	-1.97799500	1.58021500
C	-5.75941300	1.96227700	1.42376100	C	-5.49770900	-2.77399400	0.66979900
C	-5.81633500	1.31185800	0.12549900	C	-4.49861300	-3.60961000	1.22544100
C	-4.67707700	1.74331300	-0.62408500	C	-3.34430500	-3.97748000	0.46351600
C	-4.08725300	0.92831700	-1.63182600	C	-3.17779700	-3.49437200	-0.85981300
C	-2.70529800	1.12070500	-1.92072100	C	-1.83732300	-3.35326600	-1.34847700
C	-1.88957100	0.08262000	-2.46823100	C	-4.15619200	-2.61344800	-1.39916000
C	-0.51819000	0.32527000	-2.04382900	C	-5.31289600	-2.25785500	-0.64395100
C	0.43402200	-0.72267500	-1.95474200	C	-4.47725000	2.64015100	1.51631800
C	1.34084400	-0.74460800	-0.79238800	C	-3.85261500	2.55786800	0.23287700
C	1.34598100	-2.13154800	-0.22043600	C	-2.43585700	2.56847500	0.08388300
C	0.93691200	-2.00705400	1.17890700	C	-1.88157900	1.93870600	-1.06744400
C	-0.05507500	-2.86363600	1.79106300	C	-0.55000900	1.41841200	-1.08943700
C	-0.60106500	-2.41544400	3.02294900	C	0.19109300	1.31505700	0.14277800
C	-1.88159600	-2.85079100	3.47428100	C	1.05224600	0.17668900	0.31707900
C	-2.48184600	-1.82689100	4.26968900	C	0.93674100	-0.59602300	1.52380800
C	-3.88903000	-1.67423500	4.35301200	C	0.22636100	-0.10508800	2.67137600
C	-4.36718900	-0.34659700	4.71069000	C	-0.42010000	-1.05867200	3.50028800
C	-5.70027400	0.07481400	4.39226900	C	-1.56912600	-0.69696000	4.26594800
C	-5.63250600	1.39978100	3.80463400	C	-2.08756700	0.62275200	4.21229000
C	-6.96309100	0.07578400	2.42342100	C	-3.48848600	0.79085100	4.47010300
C	-6.52413700	-0.74552100	3.53585800	C	-4.25165700	1.83501100	3.83339000
C	-6.00098300	-1.97423100	3.01134800	C	-3.67766400	2.53739000	2.71026200
C	-4.73400300	-2.51744100	3.47763000	C	-2.26833500	2.46974600	2.55555800
C	-4.09043200	-3.43511500	2.60859500	C	-1.64402600	2.57866200	1.27094200
C	-2.68066300	-3.66015900	2.65490400	C	-0.40181300	1.87121900	1.30776000
C	-2.20879700	-4.03790500	1.36143700	C	-0.32272300	1.20097200	2.57974900
C	-0.89460200	-3.71573100	0.93022600	C	-1.47148200	1.56796700	3.34951700
C	-0.68622200	-3.61661700	-0.50156300	Sc	-4.75474000	-0.07972700	2.41187900
C	0.42638700	-2.91203100	-1.06129700	Sc	-0.81142900	-1.26665100	-0.22053900
C	-0.06266100	-2.07237500	-2.13714100	N	3.66477200	-1.80716900	-1.10276900
C	-1.47618900	-2.33624500	-2.30385600	N	3.44748400	-0.74718600	-1.50178400
C	-2.40328300	-1.25788600	-2.54981600	N	3.14963400	-2.70172000	-0.35661000
C	-3.75606600	-1.46529700	-2.17652100	C	3.29719800	-4.09846300	-0.76476400
C	-4.61995100	-0.38223300	-1.81874500	H	4.34443400	-4.40097500	-0.70898500
C	-5.63518900	-0.88317700	-0.94221600	H	2.90133400	-4.27642500	-1.77046400
C	-6.27558400	-0.04907700	0.01082700	H	2.72246600	-4.68021900	-0.04253900
C	-6.78187700	-0.68319000	1.20479400				

Gas phase Absolute energy = -2810.87183335 a.u. Zero-point corrected energy = -2810.400530 a.u.

Solvent phase Absolute energy = -2810.90370355 a.u.

Adduct---d---22–19

C	1.48068200	-3.24939800	-1.22465400	C	1.09778600	0.24378900	-1.15255300
C	0.13823300	-3.56877700	-1.60662900	C	0.02679800	1.18134600	-1.03656900
C	-0.68407400	-2.65130100	-2.37732600	C	-0.12666700	1.83023500	0.21703400
C	-2.04379400	-2.94234400	-2.08758400	C	-1.39668700	2.31074000	0.63704800
C	-3.07681100	-1.95358600	-2.16147500	C	-2.54180500	2.12694800	-0.18715400
C	-4.24186600	-2.15206900	-1.37230300	C	-3.81589900	2.04087200	0.46085300
C	-5.05339200	-1.06165900	-0.93503900	C	-2.40188000	1.43790100	-1.41965900
C	-5.69529800	-1.46174100	0.30830800	C	-1.11874600	0.97093300	-1.84899200
C	-6.12832700	-0.50598400	1.26303200	C	-0.74863400	-4.30949400	-0.72706000
C	-5.81483200	-0.78099400	2.65856000	C	-2.08564300	-3.96573800	-1.07074100
C	-5.22171000	0.40172800	3.25140300	C	-3.16263600	-4.02414500	-0.13276500
C	-4.01369300	0.01617500	3.91641800	C	-4.28765600	-3.18986700	-0.36162800
C	-2.78173900	0.77278200	3.74794900	C	-5.11988200	-2.73745900	0.70689500
C	-1.57862200	0.08168300	4.04881400	C	-4.71671200	-2.96261700	2.07236700
C	-0.32710600	0.46332300	3.48533500	C	-5.00834500	-1.92179400	3.03014000
C	0.51856500	-0.68019700	3.35885300	C	-3.94984500	-1.43927000	3.87962300
C	1.50805400	-0.80106700	2.34364300	C	-2.70741900	-2.14262200	4.00491000
C	1.89178900	-2.13628500	1.98379000	C	-1.54445800	-1.36012600	4.22566600
C	2.69480700	-2.47974600	0.75556300	C	-0.26695700	-1.82180400	3.79289100
C	1.85530700	-3.57668200	0.12676800	C	-0.13379100	-3.07394900	3.14268300
C	1.92316600	-1.91182100	-1.51368900	C	0.97932200	-3.22955400	2.25759700
C	2.73464000	-1.33233400	-0.35818200	C	0.89056100	-4.06953600	1.08754800
C	1.95219400	-0.08563800	-0.03221500	C	-0.40470000	-4.51000100	0.66294800
C	1.53862200	0.26493300	1.28730800	C	-1.46369300	-4.48507700	1.60766700
C	0.57975800	1.31270800	1.37851700	C	-2.83370200	-4.34441900	1.21719400
C	-0.29831100	1.45254800	2.49026500	C	-3.54944200	-3.73594700	2.29664800
C	-1.50522000	2.08344700	2.06913600	C	-2.58722400	-3.37763100	3.31374700
C	-2.74319000	1.82575000	2.71177500	C	-1.30639500	-3.83564000	2.88126400
C	-3.93891400	2.05916500	1.91389200	Sc	0.41676200	-1.90130600	0.16469000
C	-5.18387400	1.43323900	2.23999000	Sc	-3.94064000	-0.26372100	1.58126000
C	-5.75175700	0.88127500	1.02466700	N	4.85156100	-2.09319400	0.22934500
C	-4.88734600	1.24123700	-0.07948800	N	4.15316300	-2.80093400	0.96253400
C	-4.59586900	0.29152200	-1.12550300	N	4.18059900	-1.15315900	-0.45981900
C	-3.38963100	0.47883700	-1.84895300	C	4.77659000	-0.60210600	-1.65940600
C	-2.68993300	-0.61427500	-2.45455000	H	4.37315300	0.39998000	-1.82268600
C	-1.30001600	-0.27680000	-2.53655900	H	4.56778400	-1.22495900	-2.53801600
C	-0.28212800	-1.26932000	-2.52948000	H	5.85287700	-0.53610000	-1.49975700
C	1.00035400	-0.91004800	-2.01083100				

Gas phase Absolute energy = -2810.89992910 a.u. Zero-point corrected energy = -2810.426940 a.u.

Solvent phase Absolute energy = -2810.93239743 a.u.

Adduct---e1---9–10

C	-4.64051900	2.14655200	2.72166400	C	-5.26423500	0.54966600	-0.36531500
C	-3.49852200	2.88973100	2.32280500	C	-4.51927300	0.23517800	-1.55052400
C	-3.29758200	3.29321000	0.93634300	C	-4.10557100	-1.11569900	-1.71990300
C	-1.89688900	3.46018800	0.73657900	C	-2.93714900	-1.41560300	-2.46977900
C	-1.28659000	3.28551000	-0.53806300	C	-2.17288700	-0.38480800	-3.07857100
C	0.08665100	2.90877400	-0.56089500	C	-0.77604200	-0.64595500	-3.28045800
C	0.66685100	2.20321000	-1.65883700	C	-2.56609900	0.96421400	-2.88815800
C	1.78733800	1.45843700	-1.15797700	C	-3.72885800	1.26834800	-2.11197100
C	2.48138200	0.36823800	-1.91038800	C	-2.18746400	2.64256800	2.89970600
C	2.80322800	-0.92789400	-0.94755200	C	-1.21016600	3.05944600	1.94441100
C	1.92720100	-2.03735700	-1.50632100	C	0.08600900	2.47842500	1.88628700
C	1.18887700	-2.66471300	-0.46874700	C	0.77245800	2.50890600	0.63485300
C	-0.17121900	-3.11318700	-0.65469300	C	1.78716900	1.56584100	0.27687900
C	-0.94528600	-3.32511800	0.51780600	C	1.99575400	0.39919100	1.12610800
C	-2.37008700	-3.27261300	0.49618600	C	2.30830900	-0.83731400	0.48740500
C	-2.85122100	-2.82964500	1.76634100	C	1.52498600	-1.99394900	0.78588700
C	-4.05900700	-2.09381300	1.88061500	C	0.64477600	-2.04405200	1.91080500
C	-4.17821900	-1.24119800	3.05240300	C	-0.52192700	-2.84782600	1.81453900
C	-5.10031900	-0.14610100	3.08914600	C	-1.68602700	-2.54444400	2.58432600
C	-4.40914300	1.01560000	3.61261700	C	-1.69444100	-1.42307900	3.45460400
C	-5.51339500	1.66092000	1.66189300	C	-2.95903400	-0.80118000	3.71526500
C	-5.78161000	0.25235400	1.88039200	C	-3.06797600	0.61254400	3.97861100
C	-5.52934200	-0.45135900	0.65981000	C	-1.94058200	1.46699200	3.69603600
C	-4.75531000	-1.68453900	0.64242000	C	-0.67073900	0.84316400	3.57002100
C	-4.18248400	-2.04751600	-0.60365200	C	0.37709400	1.39854400	2.76768400
C	-3.03017900	-2.88162700	-0.67642200	C	1.23010200	0.33472600	2.32713100
C	-2.26723300	-2.54699200	-1.83965200	C	0.61986000	-0.89819800	2.74908900
C	-0.86776900	-2.71874400	-1.89259500	C	-0.54438200	-0.59097300	3.52165400
C	-0.14830600	-1.87715100	-2.83578500	Sc	-3.61011700	0.53455600	1.60240400
C	1.25831100	-1.60794800	-2.69243700	Sc	0.38978100	-0.48550100	-1.00481800
C	1.47753700	-0.20041400	-2.91448100	N	4.72959800	-0.25952900	-1.90582000
C	0.20555800	0.40241700	-3.23451500	N	4.27895500	-1.10674700	-1.11983300
C	-0.19185800	1.68157700	-2.69704600	N	3.84955600	0.65169700	-2.32365700
C	-1.57223600	1.97677900	-2.62370400	C	4.14241400	1.49182700	-3.46233900
C	-2.10872100	2.85059300	-1.61677600	H	3.68566400	2.47257600	-3.30670100
C	-3.46551500	2.47655900	-1.36352500	H	3.75827700	1.05655700	-4.39302900
C	-4.09986800	2.72785300	-0.12016100	H	5.22495100	1.60218500	-3.52688500
C	-5.17036000	1.83985900	0.26609700				

Gas phase Absolute energy = -2810.91264598 a.u. Zero-point corrected energy = -2810.439112 a.u.

Solvent phase Absolute energy = -2810.94464510 a.u.

Adduct---e2---10–53

C	-4.44467700	-0.48997700	5.96590800	C	-2.09972500	-3.13851100	5.79763500
C	-5.11696600	-0.76461700	4.74009200	C	-1.52820500	-3.99244600	4.80049000
C	-5.17317200	-2.10777600	4.18278500	C	-0.19492300	-3.71535900	4.38903200
C	-5.34081300	-1.97739600	2.76867000	C	0.23970400	-4.05807100	3.07073400
C	-4.87574600	-2.96573800	1.84753800	C	-0.63976600	-4.68481800	2.15232900
C	-4.58111500	-2.55073800	0.52603200	C	-0.39092100	-4.48469100	0.74824300
C	-3.62070800	-3.24851800	-0.27789800	C	-1.98778500	-4.91653400	2.54883300
C	-3.05753100	-2.30419300	-1.22154300	C	-2.42828100	-4.56320300	3.86276200
C	-1.82919800	-2.52758800	-1.83833500	C	-5.07360000	0.16757300	3.62410800
C	-0.92176100	-1.33139900	-2.15040300	C	-5.28211300	-0.58434300	2.42775200
C	0.35201300	-1.75671200	-1.40857000	C	-4.77834200	-0.16505900	1.15650500
C	0.67393500	-0.81033100	-0.39214400	C	-4.54891800	-1.15396800	0.16940800
C	1.25993100	-1.23259200	0.87664200	C	-3.55026000	-0.96984900	-0.84211800
C	1.19382000	-0.27872800	1.91964500	C	-2.67201300	0.13213000	-0.80354600
C	1.24205300	-0.66239200	3.30217400	C	-1.30787300	0.06297300	-1.47726500
C	0.53793900	0.30039200	4.08637500	C	-0.24581100	0.27160100	-0.39988900
C	-0.15067800	-0.07642200	5.26595100	C	-0.43774700	1.12460000	0.71386600
C	-1.26268000	0.77270800	5.65647000	C	0.41147000	0.92534100	1.83444000
C	-2.29172500	0.30283800	6.53628000	C	-0.00809000	1.27340700	3.15706600
C	-3.57868200	0.68458700	5.98930600	C	-1.29366300	1.82325200	3.36857300
C	-3.66945700	-1.58300000	6.53844100	C	-1.90669900	1.59568600	4.64203100
C	-2.34811600	-1.09595000	6.87498900	C	-3.33959200	1.47765700	4.79750800
C	-1.37965700	-1.99626000	6.33123600	C	-4.13613000	1.26794100	3.61337800
C	-0.21439100	-1.51563200	5.60942500	C	-3.55507700	1.61656800	2.36877500
C	0.41435100	-2.45243900	4.75421400	C	-3.93425100	0.97950200	1.14466600
C	1.18066900	-2.01701000	3.62318800	C	-2.85026900	1.08878700	0.21697500
C	1.12650300	-3.00743000	2.59253900	C	-1.73403800	1.68971700	0.92097000
C	1.25469200	-2.66627900	1.22423100	C	-2.16109000	1.98218500	2.23921700
C	0.66855200	-3.59978100	0.26666700	Sc	-2.69672800	-0.83809700	4.68228000
C	0.29760600	-3.15029600	-1.04428100	Sc	-1.10566100	-2.21904900	0.32495300
C	-1.03565400	-3.63853400	-1.33446800	N	-0.89356800	0.42764700	-3.66102600
C	-1.47453700	-4.44586500	-0.21119100	N	-1.18399200	1.02813700	-2.61959600
C	-2.81968300	-4.30615800	0.28037300	N	-0.86600800	-0.92471100	-3.54645400
C	-3.07173000	-4.66323400	1.63543500	C	-0.04763800	-1.65424400	-4.49297200
C	-4.13640200	-4.06867500	2.38018800	H	-0.13634000	-1.16448300	-5.46288500
C	-3.78735300	-4.09134800	3.76733600	H	-0.42322500	-2.67754800	-4.57130700
C	-4.31746600	-3.15050300	4.69282300	H	1.00571800	-1.67837400	-4.18483100
C	-3.51293800	-2.84565100	5.84573600				

Gas phase Absolute energy = -2810.90892429 a.u. Zero-point corrected energy = -2810.434294 a.u.

Solvent phase Absolute energy = -2810.94033857 a.u.

Adduct---e3---11–12

C	-3.86235800	1.70252300	1.81355400	C	-3.87714700	-1.71041200	0.93760600
C	-3.23306400	2.19642900	0.64593000	C	-3.15748600	-2.55791100	0.03201000
C	-3.33950800	1.51600100	-0.63200100	C	-2.16639100	-3.39838600	0.59641600
C	-2.20960500	1.89935200	-1.41677200	C	-1.04255500	-3.84250200	-0.16979600
C	-1.66366100	1.01954000	-2.39919500	C	-0.89153400	-3.39639000	-1.50504100
C	-0.28259300	1.14708700	-2.71170100	C	0.44592600	-3.28988700	-2.01749500
C	0.49732100	0.07913300	-3.27654200	C	-1.85273500	-2.50864000	-2.05596400
C	1.89234400	0.30651800	-2.91964600	C	-2.99141900	-2.09588300	-1.30510900
C	2.81546700	-0.77531500	-2.77359300	C	-1.93193100	2.83871800	0.69451200
C	3.64470400	-0.80447800	-1.59699100	C	-1.34515300	2.71224900	-0.60077900
C	3.81031800	-2.22669700	-1.02594600	C	0.07058900	2.65562500	-0.76312500
C	3.53933400	-2.08557500	0.52470200	C	0.58102400	1.96551000	-1.90441800
C	2.29839700	-2.78564700	1.08613400	C	1.89142600	1.40098000	-1.94563400
C	1.81466000	-2.29172900	2.30852800	C	2.63202800	1.30582200	-0.71446400
C	0.51068000	-2.66270500	2.77492100	C	3.41861500	0.10269300	-0.51490400
C	-0.04602800	-1.59885100	3.54457200	C	3.33807200	-0.58420200	0.71948300
C	-1.44255300	-1.40046400	3.66857900	C	2.69248900	-0.03542100	1.85771000
C	-1.86773700	-0.04765300	3.99732000	C	2.06497300	-0.93437700	2.76881400
C	-3.19178600	0.40974300	3.67577900	C	0.91731200	-0.50489400	3.48633100
C	-3.08378800	1.70889200	3.04137100	C	0.43510400	0.83007000	3.41213300
C	-4.48000900	0.38996700	1.72436700	C	-0.95146100	1.04889300	3.69431700
C	-4.05871500	-0.40887700	2.85762100	C	-1.69146000	2.09799700	3.03356800
C	-3.59250100	-1.67484200	2.36629300	C	-1.11644800	2.74716500	1.88080300
C	-2.33381300	-2.24175000	2.82963000	C	0.28711900	2.63502900	1.70644500
C	-1.73080500	-3.18428600	1.96464000	C	0.87667500	2.67529100	0.40527400
C	-0.32348000	-3.45997800	1.99197300	C	2.08913100	1.90390700	0.43966500
C	0.10971100	-3.89693700	0.70815100	C	2.18172600	1.28616500	1.73692100
C	1.42044000	-3.59022700	0.26373700	C	1.07279100	1.72947200	2.51224500
C	1.59980600	-3.52175100	-1.18021100	Sc	-2.25556900	0.12036300	1.72235000
C	2.70659300	-2.89982200	-1.78632800	Sc	1.34729800	-1.06744600	-1.19495400
C	2.25186800	-2.12396300	-2.90713900	N	5.61377600	-2.90937100	0.26175300
C	0.82761100	-2.34654600	-3.04844300	N	4.80962000	-2.57723200	1.14386600
C	-0.07456600	-1.25113500	-3.31288500	N	5.11161900	-2.86350000	-0.99750600
C	-1.41712800	-1.39443600	-2.87101500	C	6.03555200	-2.77067400	-2.10518500
C	-2.24417300	-0.27598000	-2.53825300	H	6.93462100	-3.32689000	-1.83879200
C	-3.26816500	-0.71907600	-1.64037100	H	6.30081600	-1.72957700	-2.33125600
C	-3.84605200	0.16723000	-0.69596900	H	5.58081600	-3.22491800	-2.98956400
C	-4.34520300	-0.40955600	0.52957400				

Gas phase Absolute energy = -2810.92464412 a.u. Zero-point corrected energy = -2810.449266 a.u.

Solvent phase Absolute energy = -2810.95319400 a.u.

Adduct---f1---54–53

C	-2.31392600	2.45425400	3.56173800	C	-4.00320000	1.53863600	0.60451300
C	-1.04116900	2.69711000	2.98296400	C	-3.63799200	1.05378900	-0.69506200
C	-0.89426000	3.11526100	1.60112900	C	-3.85029800	-0.32178100	-0.95282800
C	0.41286500	2.72651100	1.17083200	C	-3.05646500	-1.01858000	-1.91505900
C	0.69188200	2.42373500	-0.19455700	C	-2.02443500	-0.33968300	-2.61787500
C	1.76059400	1.52213000	-0.46564700	C	-0.90864300	-1.12175400	-3.06262200
C	1.84816700	0.74823500	-1.67058600	C	-1.77123500	1.02581200	-2.31562300
C	2.64997400	-0.43710600	-1.38602800	C	-2.57766900	1.72542400	-1.36674800
C	2.47472400	-1.65800800	-2.10472300	C	0.11761900	1.88571700	3.32119200
C	2.37759300	-2.87383300	-1.33011600	C	1.02911600	1.97026900	2.23024500
C	1.19464000	-3.57932000	-1.73445100	C	1.92988400	0.90310000	1.93101900
C	0.42762100	-3.98845600	-0.62509900	C	2.36203400	0.76455100	0.59319000
C	-0.99213100	-3.81203900	-0.59847600	C	2.81158100	-0.49055300	0.05908500
C	-1.63186100	-3.85726600	0.66863600	C	2.64049200	-1.68365000	0.81910500
C	-2.86825300	-3.19000200	0.87878300	C	2.60998900	-3.04528900	0.16115900
C	-2.93118000	-2.68892700	2.21900500	C	1.32374500	-3.96878500	0.61103000
C	-3.70207200	-1.55062400	2.56619400	C	0.55185800	-3.49148600	1.82866800
C	-3.28134300	-0.83563500	3.76227100	C	-0.84199600	-3.68860300	1.87906600
C	-3.63887000	0.53815600	3.96997700	C	-1.64615000	-2.96964400	2.82318000
C	-2.45095900	1.26061000	4.38291300	C	-1.06343300	-2.05040100	3.72399800
C	-3.45618900	2.46819900	2.66422700	C	-1.90136100	-0.99070100	4.20710400
C	-4.26384400	1.28735400	2.90398300	C	-1.36527900	0.31069200	4.50687700
C	-4.51518900	0.65114900	1.64308100	C	-0.03803200	0.64229100	4.03924500
C	-4.33921300	-0.78135200	1.47479000	C	0.81594500	-0.43405200	3.69135600
C	-4.13844300	-1.23246700	0.14252100	C	1.84471300	-0.28521100	2.70858200
C	-3.48583600	-2.46326300	-0.15366100	C	2.09893400	-1.55841800	2.10756600
C	-2.84356500	-2.36344800	-1.42462400	C	1.11465100	-2.50056600	2.64968500
C	-1.64407300	-3.06595500	-1.69206300	C	0.32824400	-1.78986500	3.60578200
C	-0.79839900	-2.52110900	-2.72539400	Sc	-2.26077600	0.63728800	2.26502100
C	0.58763900	-2.86899800	-2.81473000	Sc	0.59929600	-1.49002300	-1.01708000
C	1.36692300	-1.67523600	-3.06144100	N	3.39867900	-5.02077900	0.87936600
C	0.43180200	-0.57534100	-3.17237700	N	3.77733000	-3.89340600	0.52450000
C	0.69933600	0.69687100	-2.53845000	N	2.06558600	-5.21102300	0.83035600
C	-0.41711500	1.51416300	-2.20647600	C	1.50859100	-6.31310500	1.58766300
C	-0.38871900	2.45052200	-1.12327700	H	2.21664100	-7.14062700	1.53838500
C	-1.72928000	2.64827900	-0.65572300	H	0.56509700	-6.61624400	1.12629800
C	-2.00557600	3.01798300	0.68715400	H	1.32589700	-6.04536100	2.63516900
C	-3.27754500	2.61027400	1.23440000				

Gas phase Absolute energy = -2810.92512289 a.u. Zero-point corrected energy = -2810.449676 a.u.

Solvent phase Absolute energy = -2810.95712105 a.u.

Adduct---f2---54–12

C	-2.76668400	-0.22408900	4.41497800	C	-3.88076800	-1.65831700	1.37954900
C	-2.05760100	0.87128700	3.84652200	C	-3.51293900	-1.62315000	-0.00511200
C	-2.43171700	1.44239800	2.55842400	C	-2.83785600	-2.75566200	-0.52871100
C	-1.26808500	2.06189900	2.00889200	C	-1.93755200	-2.61482100	-1.62843400
C	-1.07161800	2.20562300	0.60521100	C	-1.70836100	-1.34832700	-2.22604400
C	0.26539600	2.30784200	0.12427000	C	-0.44562700	-1.14123100	-2.87920400
C	0.62547400	1.90421700	-1.19921500	C	-2.34920100	-0.20579400	-1.66683000
C	2.01485200	1.46914900	-1.15353400	C	-3.24539500	-0.34381700	-0.56455000
C	2.54071500	0.54773400	-2.10066700	C	-0.61785900	0.99989700	3.98148300
C	3.37031300	-0.52791300	-1.58303300	C	-0.15010100	1.78827900	2.88026600
C	2.97184700	-1.77025800	-2.18405800	C	1.16230600	1.66300900	2.35239900
C	3.02166000	-2.90763700	-1.19950100	C	1.37671200	2.03323600	0.99920700
C	1.62628900	-3.48625400	-0.99805000	C	2.42615000	1.45011200	0.22091800
C	1.36508500	-3.99427200	0.28737300	C	3.16052500	0.31290100	0.72561600
C	0.06007400	-4.39754800	0.68143500	C	3.60429200	-0.67569900	-0.18690700
C	-0.08743400	-4.25200000	2.09495600	C	3.65873300	-2.16414300	0.13581000
C	-1.34382300	-3.96780300	2.67962700	C	2.96458500	-2.47501800	1.44897700
C	-1.31367900	-3.30913200	3.97681700	C	2.06896700	-3.55159800	1.50794700
C	-2.43879300	-2.56819400	4.46708400	C	1.15675300	-3.69902500	2.59873900
C	-1.96358000	-1.29971400	4.98529600	C	1.11683900	-2.73726100	3.63808100
C	-3.76059700	-0.86592500	3.56323800	C	-0.11828400	-2.56971900	4.34718000
C	-3.55039400	-2.29895100	3.58844900	C	-0.51726500	-1.29221700	4.88784400
C	-3.52081900	-2.77564800	2.23919600	C	0.17892800	-0.10758100	4.44732800
C	-2.49280300	-3.69441900	1.77674100	C	1.45787900	-0.28934900	3.86054200
C	-2.28613900	-3.74339100	0.38177700	C	1.99741800	0.62587100	2.89443800
C	-1.02425500	-4.14837600	-0.16796800	C	2.93401200	-0.06546700	2.08374100
C	-0.81291700	-3.50947300	-1.41350400	C	2.86854200	-1.46745200	2.43355000
C	0.50098500	-3.22768900	-1.88842000	C	1.95103000	-1.59714500	3.52411900
C	0.60192400	-2.16523600	-2.88053800	Sc	-1.73140100	-1.31070400	2.79696800
C	1.85932100	-1.49637800	-3.04905700	Sc	1.20976100	-0.93345300	-1.06120300
C	1.61093500	-0.06427800	-3.02806800	N	5.03670400	-3.82139000	-0.78517700
C	0.18219200	0.15429900	-2.89290400	N	4.02736800	-3.97668400	-1.48448700
C	-0.32080900	1.19570500	-2.01744600	N	5.00261400	-2.74729100	0.03043600
C	-1.63773800	1.03880700	-1.51287500	C	5.91157500	-2.74048000	1.16062200
C	-2.03695300	1.60756800	-0.25849400	H	6.05896800	-1.70701300	1.48401500
C	-3.09278300	0.81288500	0.28701100	H	6.86321000	-3.15230400	0.82406900
C	-3.33916000	0.74480000	1.68372700	H	5.53049300	-3.33073500	2.00268700
C	-3.94478500	-0.46438200	2.18473800				

Gas phase Absolute energy = -2810.90884422 a.u. Zero-point corrected energy = -2810.434218 a.u.

Solvent phase Absolute energy = -2810.94191386 a.u.

Adduct---g---11–10

C	-6.09010900	1.36372300	2.58890900	C	-6.02891300	-2.01603100	1.58425900
C	-5.46256900	1.91577300	1.44655100	C	-5.27523500	-2.81080100	0.65655400
C	-5.54911200	1.28022900	0.14306700	C	-4.27872300	-3.65535300	1.19104600
C	-4.42477200	1.71889500	-0.62360300	C	-3.14613500	-4.05547700	0.41334600
C	-3.86165800	0.89923500	-1.63924000	C	-2.98968800	-3.54800500	-0.90182000
C	-2.47551200	1.06378200	-1.93113000	C	-1.65730500	-3.39522800	-1.39452800
C	-1.67171500	0.03159100	-2.51344100	C	-3.96550200	-2.65064700	-1.42278200
C	-0.27448000	0.26934000	-2.13287300	C	-5.10676100	-2.29117400	-0.66434300
C	0.66113100	-0.80142600	-2.04126400	C	-4.17511300	2.58477000	1.52401400
C	1.73818000	-0.83028200	-0.94810800	C	-3.57687600	2.51894700	0.22725800
C	1.66707300	-2.30447500	-0.32393500	C	-2.16382800	2.50007800	0.06648900
C	1.13196300	-2.13006900	1.07983900	C	-1.63136000	1.86202200	-1.08899500
C	0.16502800	-2.98184000	1.70638600	C	-0.29666300	1.33790300	-1.15863200
C	-0.35053700	-2.55093000	2.95897700	C	0.45704300	1.18682400	0.06702400
C	-1.63175200	-2.97059100	3.42169700	C	1.30292800	0.04843200	0.20965600
C	-2.21472000	-1.93239600	4.21996900	C	1.16248300	-0.74597700	1.41051600
C	-3.61624500	-1.76704900	4.33486500	C	0.48154600	-0.25390100	2.57598100
C	-4.06837300	-0.43033200	4.70456300	C	-0.15855100	-1.20001500	3.41653500
C	-5.39729700	0.01111300	4.40216800	C	-1.28717800	-0.81720700	4.21157600
C	-5.31354100	1.33582000	3.81697100	C	-1.78085500	0.50808400	4.17153800
C	-6.68006100	0.03933700	2.44620700	C	-3.17543600	0.69386600	4.45320600
C	-6.24428100	-0.79367300	3.54997600	C	-3.92919400	1.74967600	3.82763100
C	-5.74978400	-2.03071600	3.01462000	C	-3.36013900	2.45795500	2.70363300
C	-4.48396300	-2.59329900	3.46496200	C	-1.95286500	2.37665400	2.53464200
C	-3.85662500	-3.50517800	2.57898800	C	-1.34978600	2.48260000	1.23993900
C	-2.45507900	-3.75706100	2.60822900	C	-0.13206000	1.73796500	1.24301700
C	-2.00165300	-4.13526500	1.29774000	C	-0.05075900	1.05853100	2.50623900
C	-0.69643400	-3.82362500	0.86090600	C	-1.16169000	1.45629000	3.31183800
C	-0.50804700	-3.66447600	-0.56549700	Sc	-4.46818400	-0.18429600	2.41771100
C	0.59395000	-2.97458100	-1.12542500	Sc	-0.76875100	-1.14763200	-0.39315000
C	0.12544500	-2.13306000	-2.18680700	N	3.75932200	-1.76697900	-1.16865100
C	-1.28350200	-2.38375200	-2.35632500	N	3.14129100	-0.72147400	-1.42384400
C	-2.20901300	-1.29739100	-2.59588100	N	3.06137800	-2.68282600	-0.44609200
C	-3.54955300	-1.49187400	-2.19118000	C	3.47071100	-4.06824700	-0.53637700
C	-4.40648500	-0.40527600	-1.82231100	H	4.55363600	-4.08945400	-0.66071800
C	-5.41928100	-0.90633700	-0.94822600	H	2.99359900	-4.57979900	-1.38211500
C	-6.02675200	-0.07312100	0.02424600	H	3.20413700	-4.58136400	0.39102200
C	-6.52465700	-0.71201200	1.22356800				

Gas phase Absolute energy = -2810.92795151 a.u. Zero-point corrected energy = -2810.453461 a.u.

Solvent phase Absolute energy = -2810.95655565 a.u.

S9.3 Methyl azide additions to C_{66}^{6-}

Adduct---g---11–10

C	1.77352800	1.21180100	1.92739500	C	-0.03725500	2.83341500	1.40480300
C	2.44374700	2.21328500	2.66447500	C	-0.44581400	3.15898400	0.05517900
C	1.80965200	3.49195900	2.91182800	C	-0.45093800	4.50494200	-0.41655400
C	2.86056800	4.47619300	3.05059500	C	-0.16283100	4.74024100	-1.79305000
C	2.67467400	5.84467300	2.69083600	C	0.39981600	6.00391000	-2.22943900
C	3.81911200	6.61802100	2.31682700	C	0.67924000	7.04146200	-1.28749700
C	3.71443700	7.76521100	1.44082200	C	1.71111100	7.96821400	-1.60206200
C	4.95974800	7.88713400	0.71640800	C	0.41041100	6.79122900	0.10415600
C	5.01418100	8.53966900	-0.53381100	C	-0.15651100	5.54503000	0.53489500
C	5.96456000	8.05618100	-1.61247000	C	3.86394600	2.44424700	2.47182500
C	5.09272500	7.99874800	-2.94024500	C	4.12522900	3.83070100	2.77563500
C	5.01688300	6.54752700	-3.31297100	C	5.19267400	4.56081100	2.16268400
C	3.80398100	5.91764500	-3.72174200	C	5.08214100	5.98100300	2.04815100
C	3.82296200	4.48360500	-3.78876900	C	5.79174400	6.75227400	1.04118900
C	2.63352600	3.68839600	-3.70398600	C	6.40037500	6.05181500	-0.07118300
C	2.92815600	2.42496400	-3.09694300	C	6.41799700	6.63163600	-1.37947200
C	1.95921800	1.71192800	-2.31444000	C	5.91422600	5.82349500	-2.46176400
C	2.48516900	0.78373700	-1.33975800	C	5.85375200	4.39158500	-2.36907200
C	1.70019400	0.36965200	-0.23433700	C	4.86832100	3.72309600	-3.14772900
C	2.50895300	0.43878400	0.95878500	C	4.33682900	2.44287400	-2.74475700
C	0.46345100	1.48662000	1.39297900	C	4.76226500	1.84188400	-1.52013000
C	0.44066300	1.00772100	0.03373800	C	3.85983200	0.95630000	-0.86157600
C	-0.01041800	2.05977600	-0.80700400	C	3.83102900	0.85409800	0.57922500
C	0.67003100	2.36887600	-2.04127800	C	4.55476100	1.81093000	1.37421400
C	0.45428500	3.68692700	-2.57420700	C	5.57231300	2.57273500	0.71228000
C	1.39223600	4.31765300	-3.45487200	C	5.95827800	3.88594800	1.15067000
C	1.35652900	5.74429200	-3.27772200	C	6.45833400	4.62240200	0.02043600
C	2.50520700	6.58567200	-3.50227900	C	6.26611900	3.79455700	-1.14086600
C	2.55188000	7.82553200	-2.78149900	C	5.73976500	2.52290900	-0.72103800
C	3.75420900	8.57509400	-2.57629900	N	6.93619000	9.50127000	-3.10027800
C	3.78688700	8.84224500	-1.15879400	N	7.04041200	9.07909700	-1.93480900
C	2.52141100	8.56328700	-0.55952800	N	5.98510800	8.81408800	-3.85432600
C	2.47587700	8.03336000	0.77021000	C	5.32409400	9.65115000	-4.81804100
C	1.33800200	7.23484600	1.11493800	H	6.05110300	10.36220300	-5.24296700
C	1.40316000	6.21435000	2.12551400	H	4.91984400	9.01948800	-5.62189500
C	0.43575100	5.20078800	1.80592300	H	4.47147800	10.18277700	-4.35800600
C	0.59025300	3.83620700	2.21987500				

Gas phase Absolute energy = -2717.00013625 a.u.

S9.4 4-isopropoxyphenyl azide additions to $Sc_2@C_{66}$

TS---g---11–10

C	-6.41021100	1.03646800	2.66418800	C	-4.65245000	2.37107700	1.46613700
C	-5.86267700	1.56557600	1.46480400	C	-4.05788600	2.25675400	0.17110600
C	-5.89119600	0.82206500	0.21663700	C	-2.65346100	2.39516100	-0.02801900
C	-4.82200300	1.30808000	-0.59993800	C	-2.07197000	1.74397200	-1.15305900
C	-4.18211100	0.48598100	-1.57031500	C	-0.69557000	1.35512300	-1.18498900
C	-2.83500900	0.79190500	-1.91970300	C	0.08585600	1.40914000	0.02455700
C	-1.93587000	-0.19925300	-2.42111900	C	1.05724000	0.37277800	0.24524400
C	-0.58411700	0.20477100	-2.06236000	C	1.05341900	-0.32101700	1.50284200
C	0.46748300	-0.73920300	-1.93906000	C	0.33148400	0.17888600	2.63982900
C	1.41316400	-0.59039200	-0.81222900	C	-0.19195100	-0.77173400	3.55537500
C	1.55389800	-1.92732600	-0.14692700	C	-1.34922900	-0.47002700	4.33448000
C	1.18474600	-1.74561200	1.25351000	C	-1.99734300	0.78623700	4.20772700
C	0.30189800	-2.65029000	1.95913500	C	-3.40038300	0.83625600	4.50082400
C	-0.25108300	-2.17070500	3.17662900	C	-4.28133700	1.75389600	3.82283600
C	-1.47031700	-2.69475400	3.69928100	C	-3.81299000	2.42839400	2.63588900
C	-2.14554600	-1.68015700	4.44627200	C	-2.40872800	2.48526500	2.43683800
C	-3.55803500	-1.65755200	4.56563400	C	-1.83385000	2.56564600	1.12717800
C	-4.15511100	-0.36056700	4.84734100	C	-0.52519800	1.98741200	1.16916500
C	-5.53154100	-0.09379000	4.54957800	C	-0.34664500	1.41530900	2.47831400
C	-5.61262600	1.18696500	3.87266600	C	-1.50435100	1.72314800	3.26056700
C	-6.84465400	-0.35310200	2.63122500	Sc	-4.63486500	-0.29412600	2.54834600
C	-6.29490100	-1.04777900	3.78047600	Sc	-0.66946500	-1.28626600	-0.12532700
C	-5.66759400	-2.25323500	3.32166100	N	3.81430900	-1.36333800	-1.13165700
C	-4.34048400	-2.63784600	3.77881700	N	3.38845900	-0.36021900	-1.52798000
C	-3.63457100	-3.54754200	2.95156800	N	3.45122900	-2.31525700	-0.36322500
C	-2.20865700	-3.63128300	2.96360400	C	3.74573400	-3.65133000	-0.73465100
C	-1.73822300	-4.05067200	1.68243400	C	3.48532200	-4.62922400	0.22611600
C	-0.47391800	-3.63707200	1.18516000	C	4.18085000	-4.01201500	-2.01120700
C	-0.31669900	-3.62019600	-0.25666800	C	3.67201800	-5.96925300	-0.08725600
C	0.70260700	-2.85106900	-0.89988700	H	3.13256400	-4.32659400	1.20782100
C	0.10358900	-2.14042800	-2.01162500	C	4.38843700	-5.35180100	-2.30981100
C	-1.28063000	-2.54987500	-2.11138800	H	4.36207400	-3.24712900	-2.76069000
C	-2.31563300	-1.58483500	-2.39596200	C	4.14026000	-6.33661000	-1.35056500
C	-3.63092000	-1.89659700	-1.96516700	H	3.45595100	-6.74519200	0.63935900
C	-4.58774800	-0.87970500	-1.65107600	H	4.72342200	-5.65448000	-3.29618200
C	-5.52178700	-1.41390400	-0.70609900	O	4.28127100	-7.65750800	-1.67631900
C	-6.21572800	-0.58135200	0.21032400	C	5.56158900	-8.27247700	-1.43210000
C	-6.62423500	-1.17631600	1.46099100	H	5.40271300	-9.29270300	-1.79332800
C	-5.97518100	-2.38486300	1.90423400	C	5.89348100	-8.31565400	0.05312800
C	-5.15413700	-3.16452100	1.02256600	H	6.07123700	-7.31009500	0.44803600
C	-4.06196900	-3.85728200	1.59859500	H	5.07695200	-8.77607900	0.61645000

C	-2.89859700	-4.16322800	0.82295700	H	6.80047500	-8.90605300	0.21393900
C	-2.81747200	-3.76187200	-0.53511900	C	6.66882000	-7.62198100	-2.25000900
C	-1.51189500	-3.52845800	-1.07880300	H	6.39963900	-7.59276600	-3.30969000
C	-3.89339800	-3.02097100	-1.09894000	H	6.86470600	-6.60048500	-1.90792200
C	-5.05726100	-2.72662800	-0.32885200	H	7.59384400	-8.19650700	-2.14437600

Gas phase Absolute energy = -3195.60365385 a.u. **Solvent phase** Absolute energy = -3195.63697351 a.u.

Adduct---g---11–10

C	-5.68346500	1.17925600	3.26228700	C	-3.97630300	2.48369900	1.96830700
C	-5.26109200	1.81314400	2.07014900	C	-3.61448000	2.51348800	0.58505300
C	-5.57659700	1.26677600	0.76130700	C	-2.25065500	2.50896800	0.18185400
C	-4.60185300	1.76523200	-0.15772300	C	-1.93111300	1.95012200	-1.08847000
C	-4.22925800	1.01871100	-1.30826700	C	-0.63128200	1.44028800	-1.42821700
C	-2.91276100	1.20803200	-1.82405500	C	0.32079800	1.20530100	-0.36323600
C	-2.22864700	0.22594600	-2.61334600	C	1.16189600	0.05926600	-0.44455800
C	-0.78334800	0.44907400	-2.47149500	C	1.22948200	-0.81653900	0.70372800
C	0.14555800	-0.62651900	-2.60668900	C	0.76631400	-0.40573900	1.99960700
C	1.39297600	-0.72797200	-1.71672400	C	0.28344200	-1.40936800	2.87623100
C	1.42411600	-2.24532800	-1.19894700	C	-0.68987900	-1.08515700	3.87767500
C	1.15015300	-2.17448300	0.29211200	C	-1.17301400	0.23747600	4.01249200
C	0.29556500	-3.06775000	1.01823600	C	-2.49662500	0.39661000	4.54199600
C	0.00571200	-2.72642900	2.36772900	C	-3.33964300	1.48908600	4.13067000
C	-1.18089300	-3.18251800	3.01493800	C	-2.96998100	2.27702700	2.97652600
C	-1.61014600	-2.20292400	3.96979200	C	-1.61396000	2.21326400	2.56140400
C	-2.96901600	-2.05212100	4.33678600	C	-1.24602200	2.40924700	1.19192700
C	-3.34032300	-0.74553900	4.86784200	C	-0.05238500	1.67066700	0.93186200
C	-4.69794200	-0.29065200	4.83148300	C	0.24233200	0.90723200	2.11304100
C	-4.70713200	1.07122300	4.33298800	C	-0.70543600	1.24652300	3.12540800
C	-6.29989700	-0.13403800	3.13436300	Sc	-4.12816300	-0.35182200	2.70642900
C	-5.68617800	-1.03857200	4.08681300	Sc	-1.02812500	-1.03473000	-0.77691200
C	-5.30226600	-2.23337500	3.39059900	N	3.36980700	-1.59143400	-2.29967400
C	-3.98143000	-2.82004900	3.57636700	N	2.70439200	-0.54481100	-2.37860600
C	-3.52324800	-3.66341300	2.53385300	N	2.75907900	-2.60210400	-1.63991600
C	-2.13963900	-3.91234700	2.30408500	C	3.36197900	-3.87239600	-1.56154700
C	-1.92264700	-4.19653200	0.91197000	C	2.68196800	-4.92768500	-0.95083900
C	-0.71019300	-3.84977800	0.27926600	C	4.63742700	-4.08488100	-2.09667700
C	-0.77529000	-3.58281600	-1.14085900	C	3.27835400	-6.18177500	-0.86639200
C	0.21463500	-2.85105000	-1.83231700	H	1.68802500	-4.78696200	-0.54171600
C	-0.42064500	-1.94584900	-2.73881000	C	5.22014600	-5.34074000	-2.00728100
C	-1.83928400	-2.19336400	-2.68365100	H	5.15650200	-3.26915700	-2.58418500
C	-2.78411300	-1.09827000	-2.69084800	C	4.55291700	-6.39708800	-1.38325900
C	-4.03501700	-1.32700200	-2.07105200	H	2.74905400	-7.00967800	-0.40638600
C	-4.80706800	-0.27246900	-1.48294100	H	6.20081000	-5.51951800	-2.43603800
C	-5.65676300	-0.83762300	-0.48451200	O	5.11148400	-7.64952300	-1.35205400

C	-6.07827300	-0.07655200	0.63472300	C	5.93214000	-7.97944600	-0.21765300
C	-6.36569700	-0.79931800	1.85518600	H	6.23718800	-9.00682600	-0.43877000
C	-5.82355400	-2.12176400	2.03401200	C	5.13792100	-7.96728900	1.08196500
C	-5.24846000	-2.84679800	0.93676100	H	4.83200900	-6.95019100	1.34725500
C	-4.17964900	-3.72014300	1.23200800	H	4.24389900	-8.59108900	0.99325600
C	-3.20309500	-4.06112900	0.24558200	H	5.75329700	-8.35917800	1.89748200
C	-3.27430100	-3.46157800	-1.03761700	C	7.17272400	-7.09948700	-0.13762700
C	-2.04785400	-3.26616000	-1.73957600	H	7.71925100	-7.11765100	-1.08481500
C	-4.32038200	-2.53758200	-1.32218300	H	6.90617000	-6.06321900	0.09431200
C	-5.31037800	-2.23819200	-0.35606000	H	7.83670100	-7.46347900	0.65229000

Gas phase Absolute energy = -3195.65935786 a.u. **Solvent phase** Absolute energy = -3195.69110945 a.u.