Electronic Supplementary Material (ESI) for Polymer Chemistry.

ELECTRONIC SUPPLEMENTARY INFORMATION

The Effect of LiNTf2 on the Propagation Rate Coefficient of Methyl Methacrylate

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Table of Contents

Experimental

Materials

Methyl methacrylate (Aldrich, 99%) was passed through a column of basic alumina to remove the inhibitor. Benzoin (Aldrich, 98%) was purified by recrystallization from hot ethanol. Lithium bis(trifluoromethanesulfonimidate) ($LiNTf_2$) (Aldrich, 99%), and 2-methyl-4'-(methylthio)-2-morpholinopropiophenone (MMMP) (Aldrich, 98%) were used as received.

Pulsed Laser Polymerizations

Solutions of methyl methacrylate (MMA) containing $LiNTf_2$ (ranging from 0 to 0.10 equivalents relative to MMA) and photoinitator with concentrations between 1-2 mM were transferred to a quartz windowed vial and each sealed with a rubber septa. Each sample (of approximately 1.5 mL in volume) was purged with nitrogen for about 5 minutes. Each set of samples was allowed to equilibrate at the desired temperature in a Grant LTC1 recirculating bath. The sample vial was then subsequently placed into a copper jacketed sample holder that was temperature controlled via connection to a Lauda RL6 recirculating bath. The temperature was measured directly inside the sample using a Testo 735-2 temperature meter fitted with a 0602 0593 probe and allowed to reach thermal equilibrium for approximately 2-3 minutes. Polymerization was then initiated by laser pulsing at repetition rates of up to 25 Hz. During polymerization, temperature inside the sample was to be logged by Testo Comfort Software X35 at one second intervals and the average temperature during the polymerization was used when determining Arrhenius parameters. Laser pulsing was carried out by a Quantel Brilliant Nd-YAG operating at 355nm and at ~20 mJ/pulse with the beam positioned to illuminate the sample uniformly from the bottom of the vial. After polymerization, the sample was poured into methanol to precipitate the polymer generated. Excess methanol was decanted and the samples were dried in a miVac Quattro vacuum concentrator at 30 °C for 90 minutes. The samples are then analysed for their molecular weight distribution using SEC. Selected samples were also subjected to ^{1}H-NMR to determine triad tacticities.

Solution Density determination

In order to determine accurate concentrations of MMA in the presence of $LiNTf_2$, the density of $LiNTf_2$/MMA was determined using a Blaubrand® density bottle with a 5 cm^3 nominal volume (actual value 5.3831±0.0100 cm^3) over a range of $LiNTf_2$ concentrations (including 0.10, 0.15 and 0.20 equivalents) and for temperatures from 5 °C to 50 °C. Densities of pure MMA were calculated from the third-order polynomial taken from Stickler and Meyerhoff, *Makromol. Chem.*, 179, 2729-2745 (1978).

Molecular Weight Determination

The molecular weight distributions of the samples were determined using a Viscotek GPC Max size exclusion chromatography system fitted with a Viscotek TDA 305 triple detector array consisting of a differential viscometer (DV); right angle laser-light scattering (RALLS); low

angle laser-light scattering (LALLS); and refractive index detectors. The column set consisted of a Viscotek TGuard Organic Guard Column (10x4.6mm) and two Viscotek LT5000L Mixed Medium Organic Columns (300x7.8 mm). The system was fitted with an online solvent degasser system and eluent (THF) flowrate was set to 1mL/min and columns were held at 30°C. Calibration was carried out using PolyCAL^{TM} polymethyl methacrylate standards with M_w = 64,368 and M_n = 61,304 and M_w = 93,259 and M_n = 49,032 using OmniSEC software version 4.6.1.354.

^{1}H NMR

Tacticities of poly(methyl methacrylate) were measured on a Varian MR400 400 MHz instrument in chloroform-d at room temperature. Polymer concentrations were ~ 10-30 mg/mL and peaks at 0.85 ppm, 1.02 ppm and 1.21 ppm were assigned to *rr*, *mr*, *mm* diads respectively and integrated to determine their relative ratios.

Table S1: Results for PLP of MMA with $LiNTf_2$ at 10°C

Average T (°C) from log	[I]* (10^{-3} mol.L^{-1})	[M] (mol.L^{-1})	[$LiNTf_2$]/[M]	Laser Power (mJ/pulse)	Flashing frequency (Hz)	Time (min)	Conversion (%)	L1	L2	k_p^1 (L.mol^{-1}.s^{-1})	k_p^2 (L.mol^{-1}.s^{-1})
11	1.96	9.52	0	21	10	20	2.2	214	380	224	200
_[a]	1.96	9.53	0	18	10	20	2.4	182	389	191	204
10.1	1.96	9.53	0	21	5	40	3.7	398	740	209	194
_[a]	1.96	9.53	0	18	5	40	3.9	389	740	204	194
11	1.96	9.52	0	21	2	90	5.4	932	1736	196	182
_[a]	1.96	9.53	0	18	2	90	5.1	911	1736	191	182
11.4	1.65	9.00	0.05	23	5	40	8.5	446	890	248	247
10.9	1.65	9.00	0.05	21	5	40	9.2	478	890	266	247
11.1	1.07	9.00	0.05	21	5	40	5.6	467	870	260	242
13.0	1.65	9.00	0.05	23	8.33	30	7.3	269	489	249	226
11.8	1.65	9.00	0.05	21	8.33	30	6.8	288	575	267	266
10.9	1.07	9.00	0.05	21	8.33	30	4.3	288	545	267	266
11.1	1.65	9.00	0.05	21	10	20	8.6	224	467	248	260
11.7	1.07	9.00	0.05	21	10	20	4.0	245	512	272	285
11.9	1.65	9.00	0.05	23	10	20	6.0	219	446	243	248
10.7	1.53	8.47	0.10	20	10	10	5.8	229	489	270	289
11.2	0.81	8.47	0.10	21	10	10	2.7	257	512	304	303
10.3	1.53	8.47	0.10	20	5	20	6.5	478	850	282	251
11.6	0.81	8.47	0.10	21	5	30	10.1	536	976	317	287
10.4	1.53	8.47	0.10	20	2.5	40	11.0	890	1658	263	245
11.1	0.81	8.47	0.10	21	2.5	50	5.8	1046	1860	309	275
11	1.53	8.47	0.10	20	8.33	15	7.5	288	575	283	283
11.9	0.81	8.47	0.10	21	8.33	20	8.7	302	616	297	304

* Initiator: benzoin; [a] Indicates samples were run without the temperature probe present.

Table S2: Results of PLP of MMA with $LiNTf_2$ at 25°C

Average T (°) from log	[I] (10^{-3} mol.L^{-1})	[M] (mol.L^{-1})	[$LiNTf_2$]/[M]	Laser Power (mJ/pulse)	Flashing frequency (Hz)	Time (min)	Conversion (%)	L1	L2	k_p^1 (L.mol^{-1}.s^{-1})	k_p^2 (L.mol^{-1}.s^{-1})
25.5	1.23	9.35	0.00	20	5	10	2.4	616	1201	329	321
25.6	1.23	9.35	0.00	21	5	10	2.1	630	361	337	344
25.7	1.23	9.35	0.00	20	10	5	1.5	331	616	354	329
26.4	1.23	9.34	0.00	21	10	5	1.4	331	630	354	337
26.0	1.23	9.34	0.00	20	16.67	7	2.0	182	389	324	347
26.6	1.23	9.34	0.00	21	16.67	7	1.6	199	398	356	353
27.0	1.24	8.86	0.05	24	5	10	5.6	740	1411	418	398
25.8	0.87	8.86	0.05	21	5	5	4.1	691	1379	390	389
26.4	0.87	8.86	0.05	21	10	10	3.5	338	675	382	381
26.0	1.24	8.86	0.05	24	10	5	4.2	354	707	400	399
25.0	1.24	8.86	0.05	24	2	15	4.3	1620	3087	366	348
25.1	0.87	8.86	0.05	21	2	15	4.7	1620	3232	366	365
25.3	1.24	8.86	0.05	24	1	30	5.1	3016	6302	340	356
25.1	0.87	8.86	0.05	21	1	30	5.5	3158	6449	356	364
25.8	0.86	8.36	0.10	19	5	5	1.0	691	1379	413	412
25.3	0.88	8.35	0.10	21	5	8	3.0	724	1411	433	422
25.5	0.88	8.35	0.10	21	2	12	3.6	1736	3384	416	405
25.5	0.86	8.36	0.10	19	2	12	2.4	1658	3232	397	387
26.2	0.86	8.36	0.10	19	10	4	4.6	389	740	465	443
26.0	0.88	8.35	0.10	21	10	4	3.3	398	724	476	433
25.8	0.88	8.35	0.10	21	10	4	3.0	389	724	465	433

Initiator: benzoin

Table S3: Results of PLP of MMA with $LiNTf_2$ at 40°C

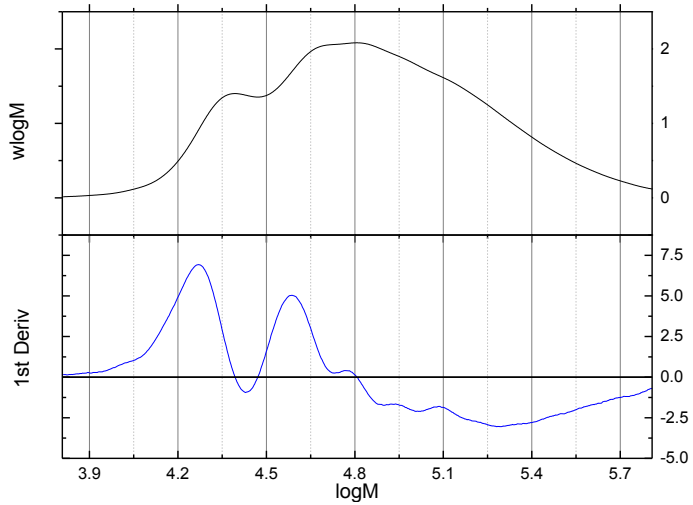
Average T (°) from log	[I] (10^{-3} mol.L^{-1})	[M] (mol.L^{-1})	[$LiNTf_2$]/[M]	Laser Power (mJ/pulse)	Flashing frequency (Hz)	Time (min)	Conversion (%)	L1	L2	k_p^1 (L.mol^{-1}.s^{-1})	k_p^2 (L.mol^{-1}.s^{-1})
40.5	1.36	9.18	0.00	22	5	5	1.7	954	1818	520	495
40.4	1.36	9.18	0.00	22	10	2	0.8	467	954	509	520
40.0	1.36	9.18	0.00	22	25	0.75	0.5	182	389	495	529
40.5	1.36	9.18	0.00	20	2	7	1.4	2341	4164	510	454
41.5	1.36	9.17	0.00	20	12.5	2	1.0	398	793	542	541
40.5	1.23	9.18	0.00	23	5	5	1.7	954	1903	520	532
41.1	1.23	9.17	0.00	23	10	2	1.2	489	976	533	532
41.7	1.25	9.16	0.00	23	25	0.75	0.7	199	398	544	542
40.8	1.11	8.71	0.05	20	5	4	2.5	999	1993	573	572
40.8	0.87	8.71	0.05	23	5	4	3.2	1070	2039	614	585
40.9	1.11	8.71	0.05	20	10	1.5	1.3	501	1022	575	587
41.2	0.87	8.71	0.05	23	10	2	1.9	549	1046	630	600
41.1	1.11	8.71	0.05	20	25	0.5	0.9	199	398	572	548
41.0	0.87	8.71	0.05	23	25	0.5	0.6	234	457	672	655
41.3	0.87	8.71	0.05	21	25	0.5	1.4	234	446	672	640
40.3	0.88	8.25	0.10	20	5	3	1.9	1201	2135	730	649
40.7	0.88	8.23	0.10	23	5	3	2.8	1095	2087	665	634
40.3	0.88	8.25	0.10	20	10	1.5	1.4	575	1121	698	681
40.8	0.88	8.25	0.10	20	10	2	3.4	536	1070	652	650
40.4	0.88	8.25	0.10	20	2	7	4.1	2396	4781	582	581
40.5	0.88	8.23	0.10	23	2	7	2.5	2509	5006	610	608
41.3	0.88	8.25	0.10	20	25	1	2.5	219	467	664	710
41.6	0.88	8.22	0.10	23	25	0.75	0.7	209	446	634	678

Table S4: Results of PLP of MMA with $LiNTf_2$ at 40°C (continued)

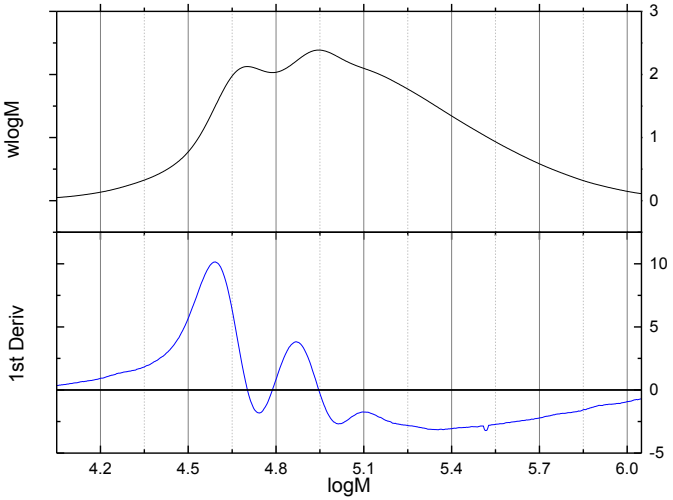
Average T (°) from log	[I] (10^{-3} mol.L^{-1})	[M] (mol.L^{-1})	[$LiNTf_2$]/[M]	Laser Power (mJ/pulse)	Flashing frequency (Hz)	Time (min)	Conversion (%)	L1	L2	k_p^1 (L.mol^{-1}.s^{-1})	k_p^2 (L.mol^{-1}.s^{-1})
41.8	1.03*	8.22	0.10	22	10	1.5	4.2	575	1095	700	667
41.5	1.03*	8.22	0.10	22	10	1.5	4.0	562	1095	684	666
40.5	1.03*	8.22	0.10	22	5	3	5.0	1121	2087	681	634
40.8	1.03*	8.22	0.10	22	5	3	5.2	1070	2037	651	620
41.2	1.03*	8.22	0.10	22	25	0.75	2.8	229	478	696	727
41.3	1.03*	8.22	0.10	22	25	0.75	3.8	214	457	650	694
39.7	0.91	7.78	0.15	20	5	3	3.4	1229	2135	790	686
40.9	0.91	7.78	0.15	20	5	5	3.0	1147	2087	737	671
41.1	0.91	7.78	0.15	20	10	3	2.2	691	1229	888	790
40.7	0.91	7.78	0.15	20	10	3	1.6	616	1147	792	737
42.1	0.91	7.78	0.15	20	25	1	1.3	245	501	788	804
42.7	0.91	7.78	0.15	20	25	1	3.8	245	512	788	823
40.9	0.91	7.78	0.15	20	2	10	5.5	2509	4892	645	629
40.8	0.91	7.78	0.15	20	2	10	7.5	2627	4892	675	629
41.4	0.91	7.78	0.15	20	5	6	6.3	1201	772	772	702

Initiator = benzoin except for * where MMMP was used.

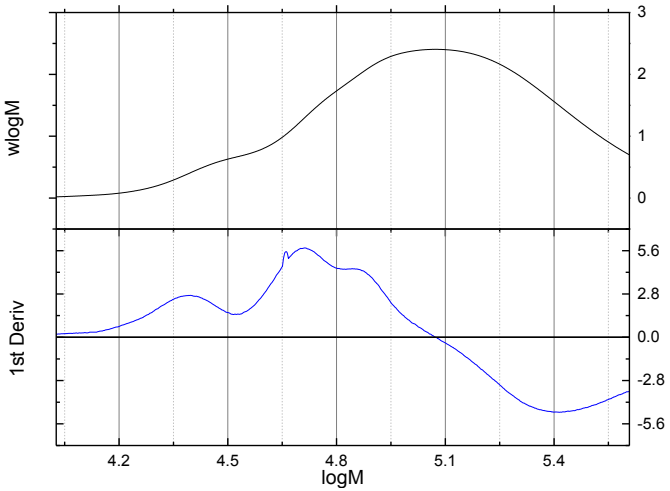
Selected Examples of PLP traces and their derivatives

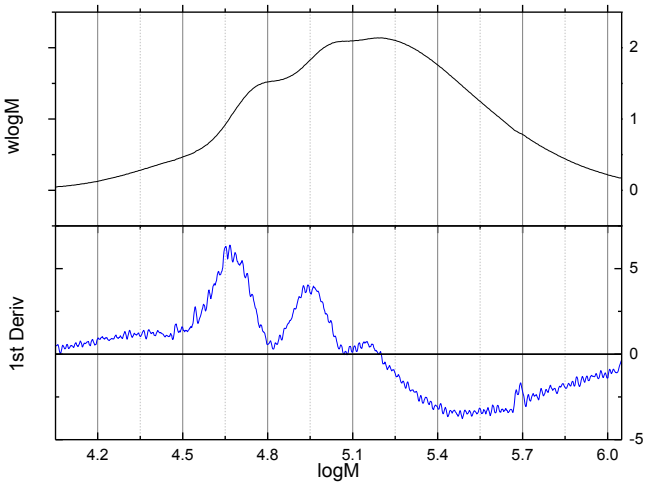


10°C, [$LiNTf_2$]/[MMA]=0, 10 Hz



10°C, [$LiNTf_2$]/[MMA]=0, 5 Hz





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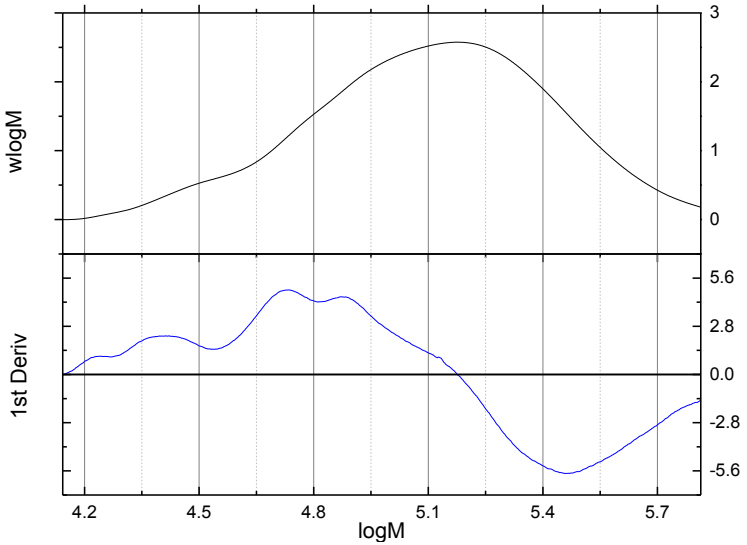

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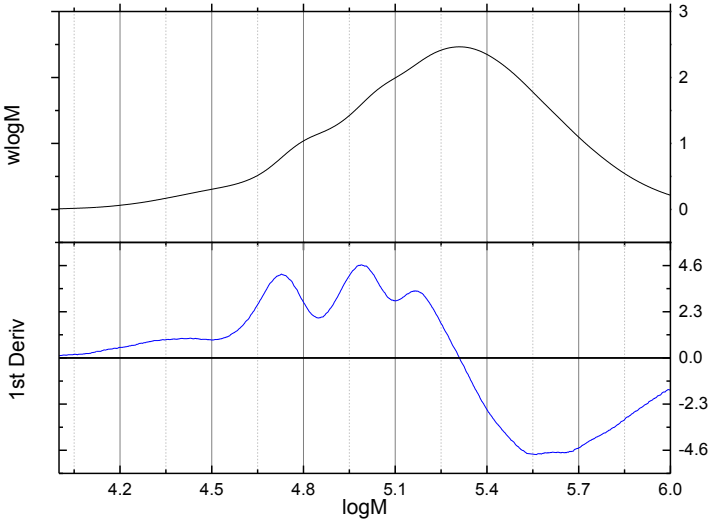
10°C, [LiNTf$_2$]/[MMA]=0.05, 5Hz



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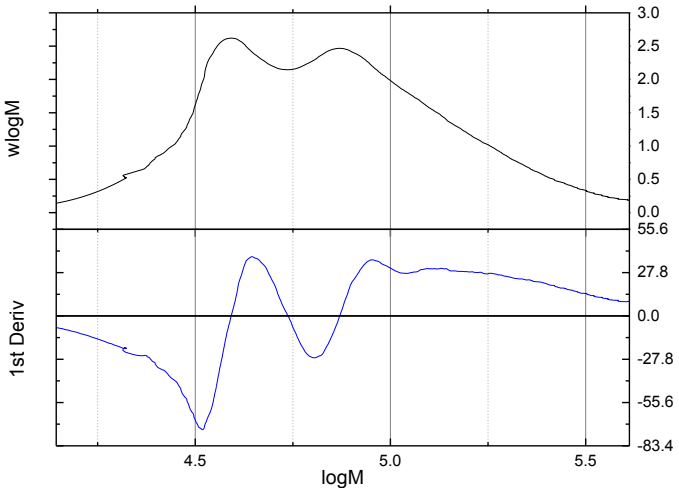

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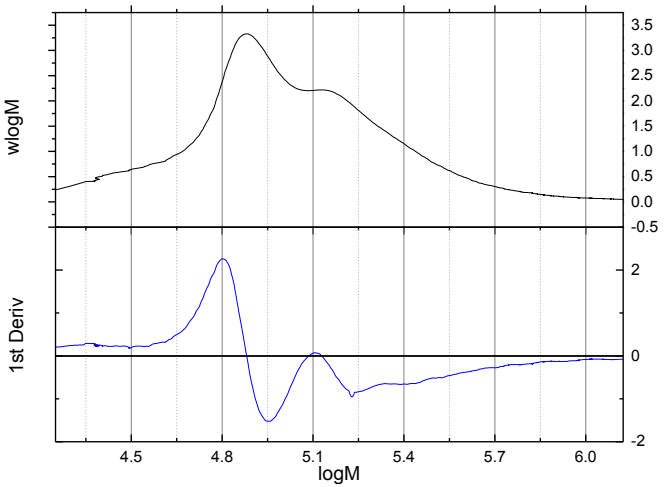

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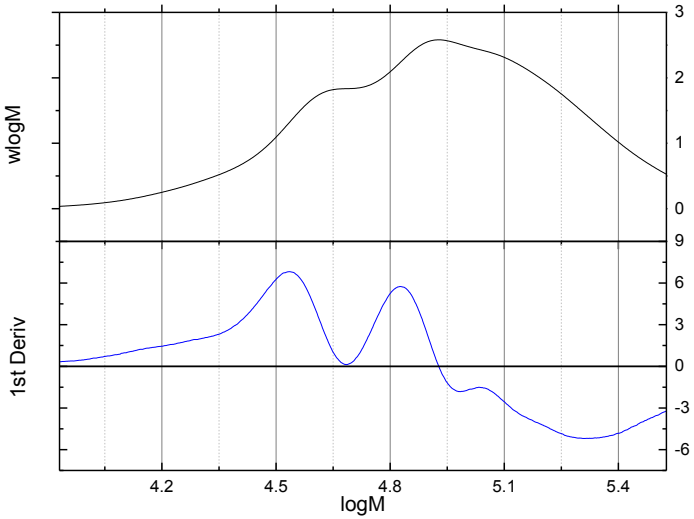

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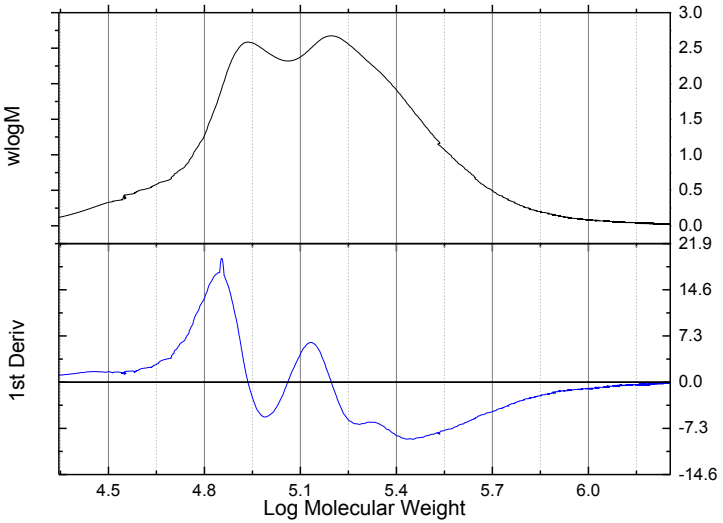

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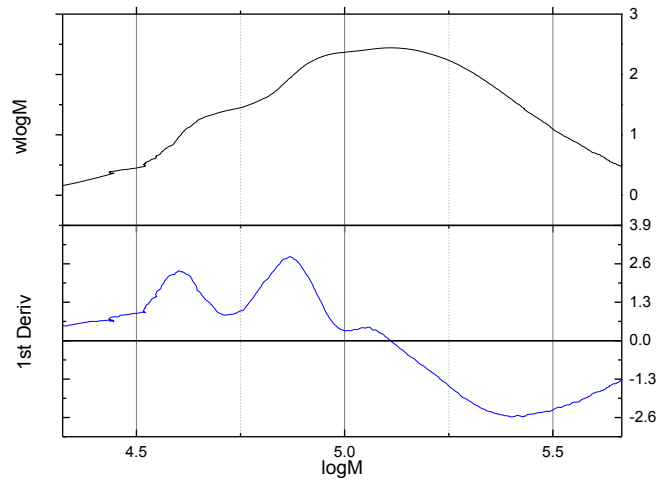

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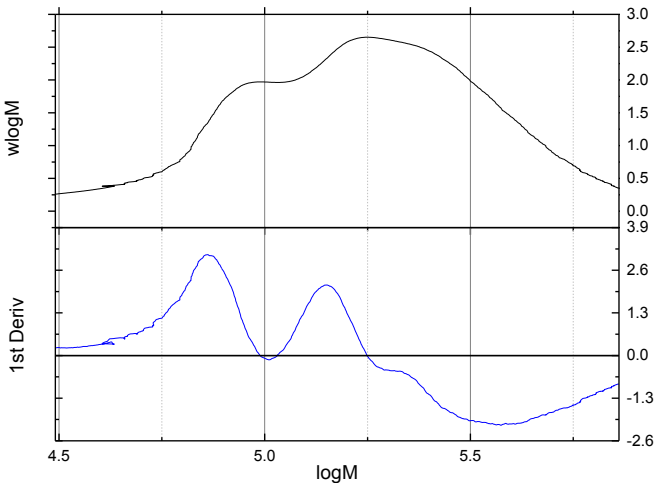

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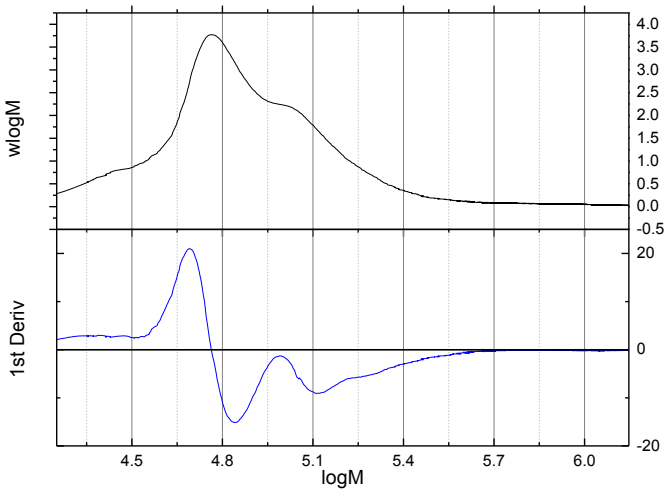

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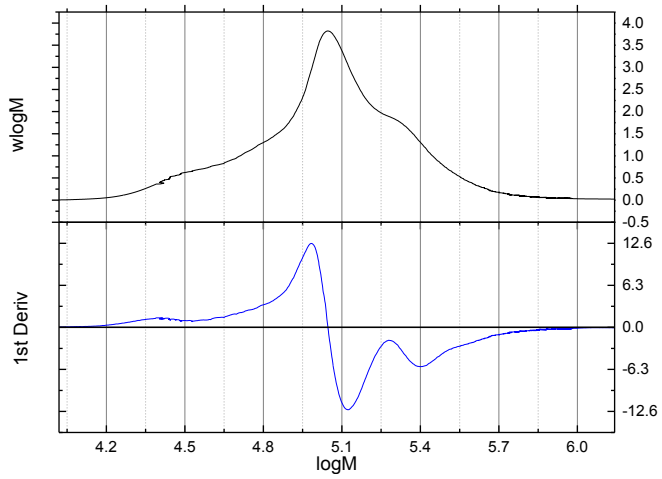

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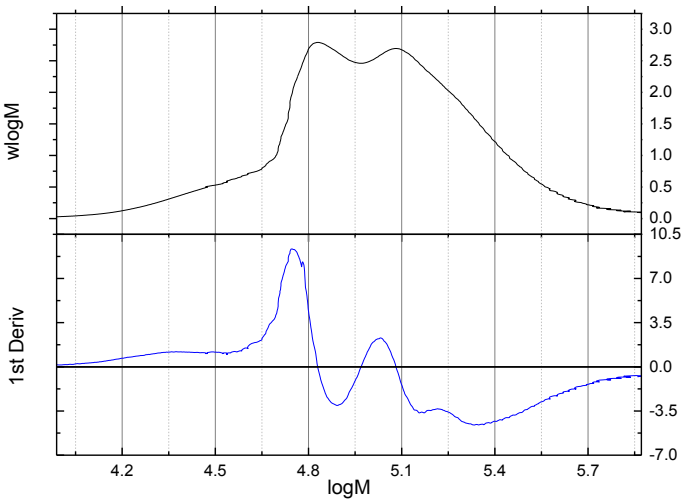

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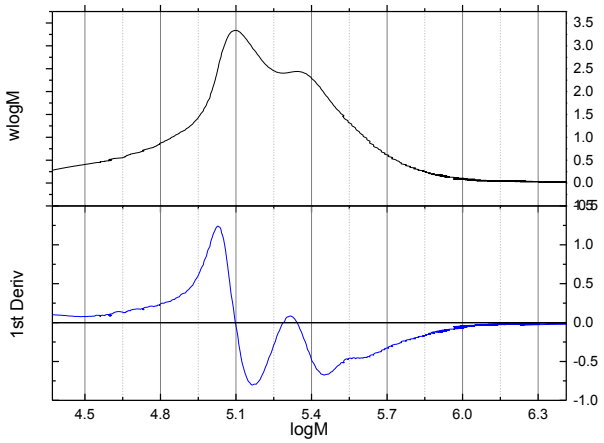
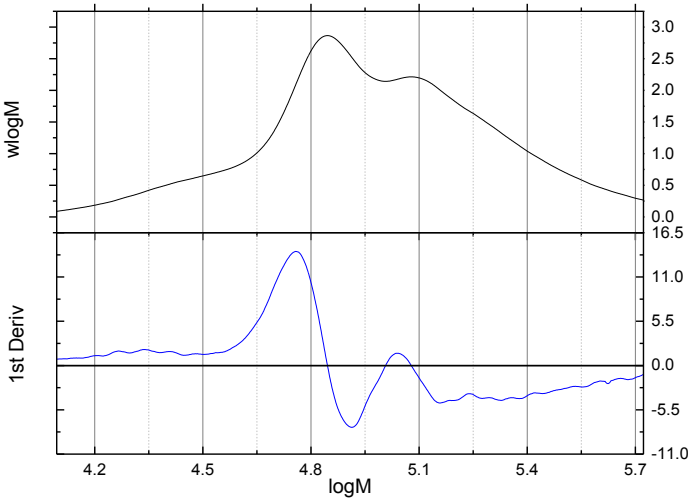


40°C, [LiNTf$_2$]/[MMA]=0.05 , 5 Hz



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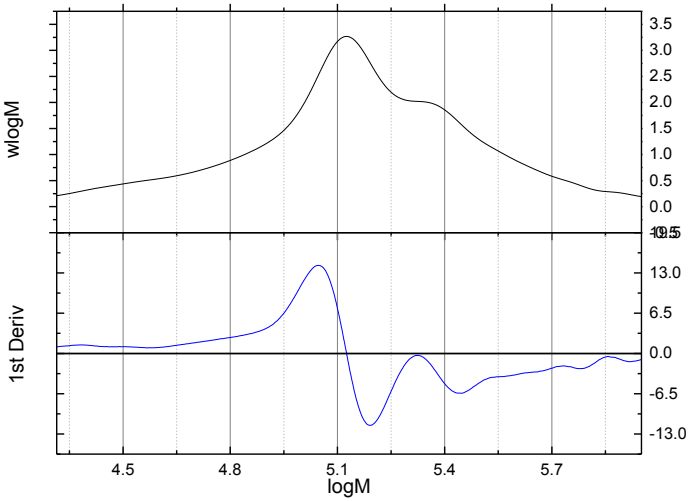

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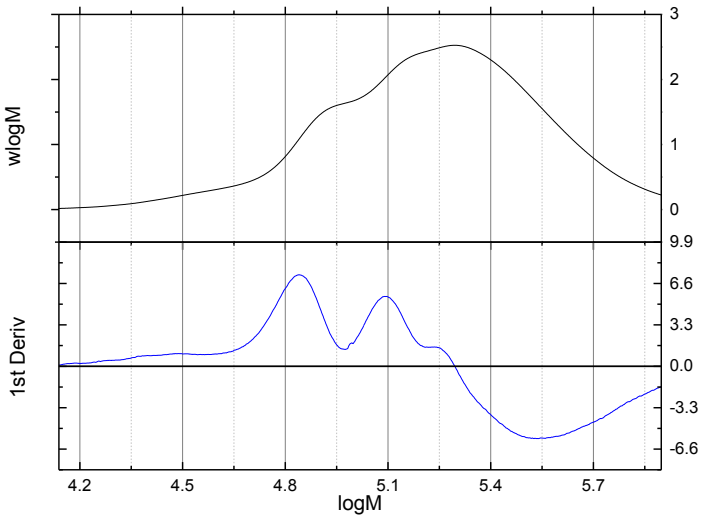

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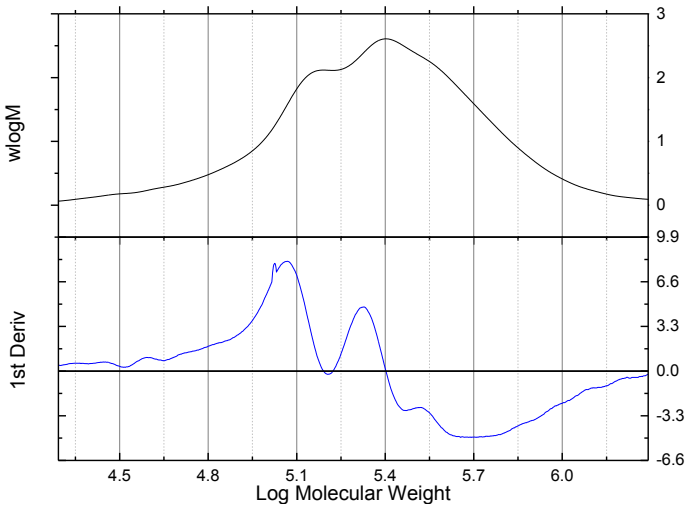

40°C, [LiNTf$_2$]/[MMA]=0.15 , 5 Hz

Details of theoretical procedures

Quantum Chemical Calculations

Standard *ab initio* molecular orbital theory and density functional theory (DFT) calculations were carried out using Gaussian 09,[1] with the exception of CCSD(T) calculations that were performed using Molpro 2009.1.[2] Calculations on radicals were performed with an unrestricted wave function except in cases designated with an "R" prefix where a restricted open-shell wave function was used. Calculations were performed at a high-level of theory, previously shown to predict accurate values for the kinetics and thermodynamics of a wide range of radical reactions, including propagation.[3,4,5] Propagating radicals were modelled as dimers to include the penultimate unit effect.[6] For all species either full systematic conformational searches (at a resolution of 120° for sp^3 centres and 180° around sp^2 centres) were carried out to ensure global - not merely local minima were located. Note that for two coordinate kinetic calculations, conformations in which a third ester group coordinated to the Li^+ were excluded (such conformations would be expected to be high energy if explicit solvating monomer was included). Chelated (κ^2) dimer radical and dimer chain complexes were found by taking respective dimer conformations, adding Li between pairs of oxygen atoms and then relaxing the geometry to the nearest minima. These conformational searches were performed in the gas-phase using M06-2X/6-31+G(d,p) and in solution phase using SMD/M06-2X/6-31+G(d,p) method with methyl propanoate (chosen to mimic bulk methyl methacrylate) as a solvent.[7] Geometries of all species were then refined *via* full optimisation at the M06-2X/6-31G+(d,p) level and frequencies were

[1] Gaussian 09, Revision **B.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, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

[2] MOLPRO 2009.1, H.-J. Werner, P. J. Knowles, G. Knizia, F. R. Manby, M. Schütz, P. Celani, T. Korona, R. Lindh, A. Mitrushenkov, G. Rauhut, K. R. Shamasundar, T. B. Adler, R. D. Amos, A. Bernhardsson, A. Berning, D. L. Cooper, M. J. O. Deegan, A. J. Dobbyn, F. Eckert, E. Goll, C. Hampel, A. Hesselmann, G. Hetzer, T. Hrenar, G. Jansen, C. Köppl, Y. Liu, A. W. Lloyd, R. A. Mata, A. J. May, S. J. McNicholas, W. Meyer, M. E. Mura, A. Nicklaß, D. P. O'Neill, P. Palmieri, D. Peng, K. Pflüger, R. Pitzer, M. Reiher, T. Shiozaki, H. Stoll, A. J. Stone, R. Tarroni, T. Thorsteinsson, M. Wang.

[3] E. I. Izgorodina and M. L. Coote, *Chem Phys*, 2006, **324**, 96-110.

[4] B. B. Noble and M. L. Coote, *Int Rev Phys Chem*, 2013, 32, 651-651.

[5] C. Y. Lin, E. I. Izgorodina and M. L. Coote, *Macromolecules*, 2010, 43, 553-560

[6] D. Bertin, P.-E. Dufils, I. Durand, D. Gigmes, B. Giovanetti, Y. Guillaneuf, S. R. A. Marque, T. Phan and P. Tordo, *Macromol. Chem. Phys.*, 2008, **209**, 220.

[7] A. V. Marenich, C. J. Cramer and D. G. Truhlar, *J Phys Chem B*, 2009, **113**, 6378-6396.

also calculated at the same level and scaled by recommended scaling factors.[8] All transition state geometries were characterized by a single imaginary frequency, other stationary points were verified as local minima – possessing no imaginary frequencies. Accurate energies for all species were then calculated using ONIOM-type method.[9] The core layer was calculated using composite high-level *ab initio* G3(MP2)-RAD method,[10] and the full system was calculated with the R(O)MP2/6-311+G(3df,2p) method. These approximations are shown in the Appendix S1.

Free energies of each species in bulk monomer solutions at 25 °C were calculated as the sum of the corresponding gas-phase free energies and the obtained free energies of solvation and included a phase change correction term $RT\ ln(RT/P)$, where R is the universal gas constant, T is the absolute temperature and P is the pressure. The entropies and thermal corrections at 25 °C (298.15 K) were calculated using standard textbook formulae[11] for the statistical thermodynamics of an ideal gas under the harmonic oscillator approximation in conjunction with the optimised geometries and scaled frequencies. Free energies of solvation in bulk monomer solutions at 25 °C were obtained using the using the popular continuum model SMD in methyl propanonate. Gaussian 09[1] was used to compute SMD solvation free energies in conjunction with the solution-phase SMD/M06-2X/6-31+G(d,p) geometries (obtained as described above) at the M06-2X/6-31+G(d,p) level of theory, and the remaining parameters were kept as default values for the corresponding solvent. Solvation free energies included a gas-phase to solution-phase geometry relaxation correction, calculated as the difference between the gas-phase energies of the gas and solution geometries (calculated at M06-2X/6-31+G(d,p)).

[8] I. M. Alecu, J. Zheng, Y. Zhao and D. G. Truhlar, *J. Chem. Theory Comput*, 2010, **6**, 2872-2887
[9] For a review, see M. L. Coote, *Macromol. Theory Simul*., 2009, **18**, 388.
[10] D. J. Henry, M. B. Sullivan and L. Radom, *J. Chem. Phys.*, 2003, **118**, 4849.
[11] J. I. Steinfeld, J. S. Francisco and W. L. Hase, *Chemical Kinetics and Dynamics*, Prentice Hall, Englewood Cliffs, 1989.

Appendix S1. Contributions to the gas and solution-phase free energies of species

Raw electronic energies, zero-point vibrational, entropic and thermal corrections, gas-phase Gibbs free energies and enthalpies at 25 °C (298.15 K), as well as free energies of solvation in bulk monomer solutions at 25 °C (where appropriate). Unless otherwise specified, units are in Hartrees. Note that solvation corrections (ΔG_{solv}) include a change of standard state from gas to solution correction.

Table S5: Monomer Binding Modes

Species	Corrections			Raw E_0					Thermochemistry	
	S (J/mol K)	TC	ZPVE	M062X/ 6-31+G(d,p)	ROMP2/ 6-31G(d)	ROMP2/ GTMP2Large	URCCSD(T)/ 6-31G(d)	G3(MP2)-RAD	$G_{gas}°$	$G_{gas}°$ (kJ /mol)
Mon Li+(O-acyl,s-trans)	397.13	0.010511	0.122793	-353.007341	-352.019518	-352.416472	-352.106399	-352.691613	-352.603407	0.0 (min)
Mon Li+(O-acyl,s-cis)	401.17	0.010610	0.122747	-353.005962	-352.018975	-352.415899	-352.105516	-352.690700	-352.602900	+ 1.3
Mon Li+(O-methoxy,s-trans)	390.04	0.010450	0.122329	-352.986719	-352.004894	-352.398359	-352.089961	-352.671687	-352.583200	+ 53.1
Mon Li+(O-methoxy,s-cis)	385.16	0.010112	0.122731	-352.982965	-351.998058	-352.394006	-352.084089	-352.668297	-352.579192	+ 63.6
Mon Li+(O,O' bis,s-trans)	393.75	0.010551	0.122489	-352.996812	-352.012957	-352.407190	-352.099044	-352.681537	-352.593212	+ 26.8
Mon Li+(O,O' bis,s-cis)	388.90	0.010358	0.122837	-352.996360	-352.011468	-352.405742	-352.097801	-352.680335	-352.591303	+ 31.8

Table S6: Ester Binding

Species	Corrections			Raw E_0						Thermochemistry	
	S (J/mol K)	TC	ZPVE	M062X/ 6-31+G(d,p)	ROMP2/ 6-31G(d)	ROMP2/ GTMP2Large	URCCSD(T)/ 6-31G(d)	G3(MP2)-RAD	ONIOM correction	$H_{gas}°$ (G3MP2-RAD)	$H_{gas}°$ (ONIOM)
Li+	133.04	0.002360	0.000000	-7.281049	-7.235536	-7.235840	-7.235537	-7.237728	0.000000	-7.235367	-7.233479
H•	114.61	0.002360	0.000000		-0.498233	-0.499818	-0.498233	-0.501706	0.000000	-0.499345	-0.497457
Rad	402.49	0.010106	0.129632	-346.226780	-345.265700	-345.675554	-345.355389	-345.957472	0.000000	-345.817734	-345.535817
Mon	365.55	0.009021	0.120680	-345.650467	-344.705919	-345.108544	-344.791742	-345.382627	0.000000	-345.252925	-344.978842
Chain	403.51	0.010974	0.170359	-386.174358	-385.076833	-385.549491	-385.182053	-385.880623	0.000000	-385.699290	-385.368158
Rad-H	379.50	0.009624	0.143385	-346.876221	-345.906916	-346.327572	-345.996934	-346.615264	0.000000	-346.462255	-346.174564
Rad Li+	431.37	0.011604	0.131964	-353.588729	-352.583250	-352.988070	-352.673792	-353.270840	0.000000	-353.127272	-352.844501
Mon Li+	397.13	0.010511	0.122793	-353.007341	-352.019518	-352.416472	-352.106399	-352.691613	0.000000	-352.558309	-352.283168
Chain Li+	424.05	0.012224	0.172807	-393.533889	-392.393093	-392.860263	-392.499294	-393.192376	0.000000	-393.007345	-392.675232
Rad-H Li+	404.08	0.010997	0.145567	-354.234246	-353.221607	-353.636739	-353.312632	-353.925437	0.000000	-353.768874	-353.480176
Rad Li+(Mon)	687.27	0.021495	0.254146	-699.297461	-697.351233	-698.152748	-697.528633	-698.710863	0.000000	-698.435222	-697.877107
Mon Li+(Mon)	650.92	0.020524	0.244963	-698.716905	-696.789046	-697.582521	-696.962682	-698.132677	0.000000	-697.867189	-697.317033
Chain Li+(Mon)	682.54	0.022341	0.294887	-739.242483	-737.161807	-738.025365	-737.354910	-738.632640	0.000000	-738.315412	-737.708137
Rad-H Li+(Mon)	666.06	0.020991	0.267846	-699.943406	-697.990795	-698.802311	-698.168701	-699.366361	0.000000	-699.077524	-698.513474
Rad Li+$(Mon)_2$	870.06	0.030810	0.376945	-1044.988358	-1042.102670	-1043.304484	-	-	-0.000226	-	-1042.896955
Mon Li+$(Mon)_2$	843.60	0.029929	0.367651	-1044.408496	-1041.539985	-1042.734293	-	-	-0.000102	-	-1042.336814
Chain Li+$(Mon)_2$	870.96	0.031775	0.417521	-1084.933427	-1081.911732	-1083.176511	-	-	-0.000171	-	-1082.727387
Rad-H Li+$(Mon)_2$	860.23	0.030513	0.390361	-1045.634396	-1042.741172	-1043.953490	-	-	-0.000387	-	-1043.533004
Rad Li+$(Mon)_3$	1049.96	0.040332	0.498962	-1390.669602	-1386.841402	-1388.446459	-	-	-0.000226	-	-1387.907392
Mon Li+$(Mon)_3$	1014.60	0.039283	0.489922	-1390.090597	-1386.279804	-1387.877468	-	-	-0.000387	-	-1387.348649
Chain Li+$(Mon)_3$	1042.96	0.041138	0.539798	-1430.615225	-1426.650540	-1428.318990	-	-	-0.000171	-	-1427.738226
Rad-H Li+$(Mon)_3$	1028.13	0.039906	0.512553	-1391.316336	-1387.480239	-1389.096235	-	-	-0.000102	-	-1388.543877

Table S7: Ester Binding (continued)

Absolute gas-phase binding enthalpies of unimeric models to $Li^+(Mon)_n$ and the methine C-H BDE of complexed Methyl isobutyrate.

Model[a]	ΔH_{bind} (25 °C, kJ /mol)				BDE[c] (25 °C, kJ /mol)
	Rad	Chain	Mon	Rad-H[b]	
n = 0	- 194.7	- 190.8	- 183.8	- 187.1	+ 373.5
n = 1	- 155.4	- 151.8	- 146.9	- 149.5	+ 375.3
n = 2	- 115.8	- 110.8	- 107.5	- 108.7	+ 374.1
n = 3	- 91.3	- 87.3	- 86.6	- 85.3	+ 376.0
				ref[d]	+ 381.2

[a] Here *n* is the number of solvating MMA monomer units.
[b] Rad-H is Methyl isobutyrate.
[c] BDE the calculated methine C-H Bond Dissociation Energy of Methyl isobutyrate complexed with $Li^+(Mon)_n$.
[d] ref is the calculated methine C-H Bond Dissociation Energy of unbound Methyl isobutyrate for reference.

Table S8: Polymer Binding Selectivity

Species	Corrections			Raw E_0						Solvation corrections	
	S (J/mol K)	TC	ZPVE	M062X/ 6-31+G(d,p)	ROMP2/ 6-31G(d)	ROMP2/ GTMP2Large	URCCSD(T)/ 6-31G(d)	G3(MP2)-RAD	ONIOM correction	E_0(sol)	ΔG_{sov}
Li+	133.04	0.002360	0.000000	-7.281049	-7.235536	-7.235840	-7.235537	-7.237728	0.000000	-7.401298	-0.117238
Mon	365.55	0.009021	0.120680	-345.650467	-344.705919	-345.108544	-345.382627	-345.382627	0.000000	-345.657949	-0.004470
Mon Li+	397.13	0.010511	0.122793	-353.007341	-352.019518	-352.416472	-352.106399	-352.691613	0.000000	-353.091686	-0.081333
Di-rad	561.66	0.017949	0.255394	-691.918224	-690.016848	-690.828968	-690.187433	-691.380042	0.000000	-691.932556	-0.011321
Di-rad[a]	548.32	0.017705	0.255616	-691.917817	-690.016456	-690.828553	-690.187048	-691.379634	0.000000	-691.932809	-0.011980
Di-chain	559.07	0.018848	0.296065	-731.862792	-729.824394	-730.700814	-730.010062	-731.300654	0.000000	-731.877619	-0.011815
Di-rad Li+	566.038	0.018670	0.259167	-699.321002	-697.376729	-698.179311	-697.549548	-698.732619	-0.000346	-699.391119	-0.067105
Di-chain Li+	572.15	0.019912	0.299315	-739.260616	-737.180729	-738.046393	-737.368577	-738.648413	-0.000292	-739.331264	-0.067636
Mon Li+(Mon)	650.92	0.020524	0.244963	-698.716905	-696.789046	-697.582521	-696.962682	-698.132677	-0.000102	-698.781283	-0.061366
Di-rad Li+(Mon)	793.91	0.028593	0.381190	-1045.016392	-1042.133751	-1043.334147	-	-	-0.000346	-1045.077476	-0.058072
Di-chain Li+(Mon)	789.04	0.029634	0.421595	-1084.957300	-1081.938455	-1083.202180	-	-	-0.000292	-1085.018984	-0.058672
Mon Li+$(Mon)_2$	843.60	0.029929	0.367651	-1044.408496	-1041.539985	-1042.734293	-	-	-0.000102	-1044.467097	-0.055590
Di-rad Li+$(Mon)_2$	991.61	0.038380	0.503127	-1390.697892	-1386.875184	-1388.477757	-	-	-0.000346	-1390.757751	-0.056848
Di-chain Li+$(Mon)_2$	980.39	0.039131	0.543877	-1430.641145	-1426.680665	-1428.347338	-	-	-0.000292	-1430.701013	-0.056856
Mon Li+$(Mon)_3$	1014.60	0.039283	0.489922	-1390.090597	-1386.279804	-1387.877468	-	-	-0.000102	-1390.147858	-0.054248
Di-rad Li+$(Mon)_3$	1174.77	0.047837	0.625017	-1736.364628	-1731.596189	-1733.604941	-	-	-0.000226	-1736.427593	-0.059952

[a] is the precursor dimer conformation for chelation.

Table S9: Polymer Binding Selectivity (continued)

Species	Gas Thermochemistry				Solution Thermochemistry	
	$H_{gas}°$ (G3MP2-RAD)	$H_{gas}°$ (ONIOM)	$G_{gas}°$ (G3MP2-RAD)	$G_{gas}°$ (ONIOM)	$G_{sol}°$ (G3MP2-RAD)	$G_{sol}°$ (ONIOM)
Li+	-7.235367	-7.233479	-7.250475	-7.248587	-7.367713	-7.365825
Mon	-345.252925	-344.978842	-345.294437	-345.020354	-345.298907	-345.024824
Mon Li+	-352.558309	-352.283168	-352.603407	-352.328265	-352.684740	-352.409598
Di-rad	-691.106699	-690.555625	-691.170481	-690.619406	-691.181801	-690.630727
Di-rad[a]	-691.106313	-690.555233	-691.168580	-690.617500	-691.180560	-690.629480
Di-chain	-730.985741	-730.385900	-731.049228	-730.449388	-731.061043	-730.461203
Di-rad Li+	-698.454783	-697.901820	-698.519061	-697.966099	-698.586166	-698.033204
Di-chain Li+	-738.329186	-737.727458	-738.394159	-737.792431	-738.461795	-737.860067
Mon Li+(Mon)	-697.867189	-697.317135	-697.941107	-697.391052	-698.002472	-697.452418
Di-rad Li+(Mon)	-	-1042.924710	-	-1043.014865	-	-1043.072937
Di-chain Li+(Mon)	-	-1082.751243	-	-1082.840845	-	-1082.899517
Mon $Li+(Mon)_2$	-	-1042.336814	-	-1042.432613	-	-1042.488203
Di-rad $Li+(Mon)_2$	-	-1387.936596	-	-1388.049203	-	-1388.106051
Di-chain $Li+(Mon)_2$	-	-1427.764621	-	-1427.875954	-	-1427.932810
Mon $Li+(Mon)_3$	-	-1387.348364	-	-1387.463581	-	-1387.517830
Di-rad $Li+(Mon)_3$	-	-1732.932313	-	-1733.065719	-	-1733.125672

Table S10: Polymer Binding Selectivity (continued)

Absolute (and relative) binding enthalpies and free energies of $Li^+(Mon)_n$ to the polymer terminus, mid-chain segment and $monomer_{(2)}$.

Model	ΔH_{bind} (gas, 25 °C, kJ /mol)			ΔG_{bind} (gas, 25 °C, kJ /mol)			ΔG_{bind} (sol, 25 °C, kJ /mol)		
	Terminus	Chain	Monomer	Terminus	Chain	Monomer	Terminus	Chain	Monomer
n = 0	-295.9 (+ 34.8)	-283.8 (+ 46.9)	-330.7 (0, min)	-257.6 (+ 9.6)	-248.0 (+ 19.2)	-267.2 (0, min)	-96.2 (+ 0.8)	-86.7 (+ 10.3)	-97.0 (0, min)
n = 1	-225.6 (+ 26.4)	-215.7 (+ 36.3)	-252.0 (0, min)	-176.4 (0, min)	-165.9 (+ 10.5)	-167.1 (+ 9.3)	-85.6 (0, min)	-75.4 (+ 10.2)	-76.0 (+ 9.6)
n = 2	-167.6 (+ 25.5)	-161.7 (+ 31.4)	-193.1 (0, min)	-101.7 (0, min)	-93.2 (+ 8.5)	-83.5 (+ 18.2)	-60.1 (0, min)	-50.4 (+ 9.8)	-41.4 (+ 18.8)

Table S11: Pro-meso/ Pro-racemo Selectivity

Species	Corrections			Raw E_0			Solvation corrections		Thermochemistry
	S (J/mol K)	TC	ZPVE	M062X/ 6-31+G(d,p)	ROMP2/ 6-31G(d)	ROMP2/ GTMP2Large	E_0(sol)	ΔG_{sov}	G_{sol}
Tri-rad (pro-r)	719.80	0.026033	0.380880	-1037.606432	-1034.764454	-1035.980584	-1037.626851	-0.017407	-1035.672817
Tri-rad (pro-m)	712.47	0.025889	0.381051	-1037.605387	-1034.762934	-1035.979624	-1037.626181	-0.017783	-1035.671374
Tri-rad (pro-r) $Li+(Mon)_2$	1140.82	0.046424	0.628257	-1736.386913	-1731.623597	-1733.630255	-1736.452753	-0.062828	-1733.147951
Tri-rad (pro-m) $Li+(Mon)_2$	1141.35	0.046345	0.628423	-1736.388550	-1731.625204	-1733.632246	-1736.454464	-0.062903	-1733.149992

Table S12: Kinetic Pathways

Note: The rad-mon pathways had different lowest energy TS conformations in gas and solution, as indicated by gas and sol suffixes, respectively. The other two pathways had the same lowest energy TS conformations in both phases.

Species	Corrections			Raw E_0					
	S (J/mol K)	TC	ZPVE	M062X/ 6-31+G(d,p)	ROMP2/ 6-31G(d)	ROMP2/ GTMP2Large	URCCSD(T)/ 6-31G(d)	G3(MP2)-RAD	ONIOM correction
Rad Li+(Mon)	687.27	0.021495	0.254146	-699.297461	-697.351233	-698.152748	-697.528633	-698.710863	-
Di-rad Li+TS (rad-monC)	572.38	0.019130	0.255354	-699.279032	-697.334056	-698.139648	-697.508046	-698.694128	-
Mon Li+	397.13	0.010511	0.122793	-353.007341	-352.019518	-352.416472	-352.106399	-352.691613	-
Rad	402.49	0.010106	0.129632	-346.226780	-345.265700	-345.675554	-345.355389	-345.957472	-
Di-rad Li+TS (monC)	593.35	0.019701	0.254196	-699.240349	-697.291314	-698.101655	-697.465342	-698.656172	-
Rad Li+	431.37	0.011604	0.131964	-353.588729	-352.583250	-352.988070	-352.673792	-353.270840	-
mono	365.55	0.009021	0.120680	-345.650467	-344.705919	-345.108544	-345.382627	-345.382627	-
Di-rad Li+TS (radC)	600.11	0.019808	0.254406	-699.239396	-697.293412	-698.103910	-697.465611	-698.656597	-
Di-rad Li+ (Mon) (rad-monC)	788.18	0.028783	0.380528	-1044.995058	-1042.107682	-1043.313107	-	-	-
Tri-rad Li+TS (rad-monC)gas	741.03	0.027252	0.380929	-1044.971701	-1042.086775	-1043.295781	-	-	0.003636
Tri-rad Li+TS (rad-monC)sol	733.91	0.027306	0.380685	-1044.969712	-1042.086017	-1043.294734	-	-	0.003636
Mon Li+(Mon)	650.92	0.020524	0.244963	-698.716905	-696.789046	-697.582521	-	-	-
Di-rad	561.66	0.017949	0.255394	-691.918224	-690.016848	-690.828968	-	-	-
Tri-rad Li+TS (monC) Mon	952.83	0.037210	0.502711	-1390.646269	-1386.816585	-1388.429280	-	-	0.002542
Di-rad Li+	566.04	0.018670	0.259167	-699.321002	-697.376729	-698.179311	-	-	-
Tri-rad Li+TS (radC)	757.43	0.027335	0.381186	-1044.965439	-1042.082060	-1043.291862	-	-	0.004166

Table S13: Kinetic Pathways (continued)

Species	Solvation corrections		Thermochemistry		
	E_0(sol)	ΔG_{sov}	H_{gas}° (ONIOM)	G_{gas}° (ONIOM)	G_{sol}° (ONIOM)
Rad Li+(Mon)	-	-	-697.877107	-697.9551526	-
Di-rad Li+TS (rad-monC)	-	-	-697.865165	-697.9301635	-
Mon Li+	-	-	-352.283168	-352.3282652	-
Rad	-	-	-345.535817	-345.5815228	-
Di-rad Li+TS (monC)	-	-	-697.827757	-697.895138	-
Rad Li+	-	-	-352.844501	-352.8934877	-
mono	-345.657949	-0.004470	-344.978842	-345.0203539	-345.024824
Di-rad Li+TS (radC)	-	-	-697.829697	-697.897845	-
Di-rad Li+ (Mon) (rad-monC)	-1045.062014	-0.063944	-1042.903796	-1042.993301	-1043.057245
Tri-rad Li+TS (rad-monC)gas	-1045.046512	-0.071799	-1042.883964	-1042.968115	-1043.039914
Tri-rad Li+TS (rad-monC)sol	-1045.046266	-0.073543	-1042.883106	-1042.966449	-1043.039991
Mon Li+(Mon)	-698.781283	-0.061366	-697.317033	-697.3909508	-697.452316
Di-rad	-691.932556	-0.011321	-690.555625	-690.6194062	-690.630727
Tri-rad Li+TS (monC) Mon	-1390.7172	-0.067894	-1387.886816	-1387.995018	-1388.062912
Di-rad Li+	-699.391119	-0.067105	-697.901475	-697.9657534	-698.032858
Tri-rad Li+TS (radC)	-1045.0409	-0.072477	-1042.879175	-1042.965188	-1043.037666

Appendix S2. Geometries of all the species in the present work

Note: All geometries had either no imaginary frequencies, or in the case of transitions states, 1 imaginary frequency.

Monomer Binding Mode

Mon Li+(O-acyl,s-trans)

1\1\GINC-V1483\Freq\RM062X\6-31+G(d,p)\C5H8Li1O2(1+)\BXN501\11-Dec-2012\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) SCF=tight Freq=(noraman) maxdisk=268435456\\MMA_mono_Li+.freq\\1,1\C,-0.0106651276,0.,-0.0245638821\O,0.0267947513,0.,1.419256883\C,1.1907636375,0.,2.0026318334\O,2.2498768662,0.,1.3506088875\C,1.1853589852,0.,3.4837958155\C,0.0248683809,0.,4.1479397458\H,-0.925051572,0.,3.6248149863\H,0.0053717026,0.,5.2331034087\C,2.5400414102,0.,4.1393280454\H,2.4449055439,0.,5.2255722271\H,3.1129013702,-0.8986068948,3.8726835657\H,3.1129013702,0.8986068948,3.8726835657\H,-1.0668571012,0.,-0.2786453868\H,0.4826945735,-0.8956739282,-0.4025648654\H,0.4826945735,0.8956739282,-0.4025648654\Li,3.9927010079,0.,1.6305373655\\Version=EM64L-G09RevA.02\State=1-A'\HF=-353.0073407\RMSD=7.674e-09\RMSF=1.275e-05\ZeroPoint=0.1269835\Thermal=0.1364259\Dipole=2.8976212,0.,-0.4728603\PG=CS [SG(C5H8Li1O2),X(H4)]\\@

Mon Li+(O-acyl,s-cis)

1\1\GINC-V1369\Freq\RM062X\6-31+G(d,p)\C5H8Li1O2(1+)\BXN501\13-Jul-2012\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) SCF=tight Freq=(noraman) maxdisk=268435456\\MMA_Li+.b2.M062X.freq\\1,1\C,0.0956214344,-0.1309618584,0.0581753948\O,0.0815141717,-0.070122964,1.4957419761\C,1.2165348525,-0.0019323049,2.1373240729\O,2.3038310516,0.0116399788,1.5339057595\C,1.0583109766,0.0549535555,3.6104939347\C,2.1678559081,0.1260598379,4.3532740513\H,3.1560450405,0.1424111703,3.9068746568\H,2.1106671735,0.1698796149,5.4356258916\C,-0.3382693564,0.0285676134,4.1658480968\H,-0.92381971,0.8740444394,3.7955676153\H,-0.3062511185,0.0760271797,5.2545572252\H,-0.8608776764,-0.8848674709,3.8703612168\H,-0.9494208111,-0.1818505598,-0.2348431318\H,0.6301070987,-1.0246296533,-0.2670539285\H,0.5641853488,0.7686199488,-0.3434524827\Li,3.8987786208,0.0412319262,0.8545292308\\Version=EM64L-G09RevA.02\State=1-A\HF=-353.0059615\RMSD=2.466e-09\RMSF=4.105e-06\ZeroPoint=0.1269353\Thermal=0.1364773\Dipole=3.2479843,0.0350298,-1.9611043\PG=C01 [X(C5H8Li1O2)]\\@

Mon Li+(O-methoxy,s-trans)

1\1\GINC-R178\Freq\RM062X\6-31+G(d,p)\C5H8Li1O2(1+)\ROOT\22-Oct-2013\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) SCF=tight Freq=(noraman) maxdisk=268435456\\MMA_mono_Li+.O-CH3.s-trans.freq\\1,1\C,0.0442850733,0.1181377699,-0.0812824589\O,0.1074353003,0.3248625303,1.3601382003\C,1.2200319954,-0.2195016215,1.976579075\O,2.1025221695,-0.7361399832,1.3662299326\C,1.1695590351,-0.0242324806,3.466873278\C,0.0063693674,-0.1950284932,4.1193750596\H,-0.8900927143,-0.557141252,3.6117687092\H,-0.0425430164,-0.1164346332,5.2009353071\C,2.4928295818,0.244334342,4.116311381\H,2.3836665623,0.362025409,5.1943464889\H,3.1595304574,-0.5993165227,3.9118655288\H,2.9710948001,1.1341621008,3.6969398859\H,-0.8841290788,0.5800850212,-0.4090573929\H,0.0419468438,-0.952047746,-0.2829325477\H,0.9095214833,0.5875825115,-0.54766484\Li,-0.7203279981,1.4609936373,2.6024005866\\Version=ES64L-G09RevD.01\State=1-A\HF=-352.9867186\RMSD=6.724e-09\RMSF=1.281e-05\ZeroPoint=0.1265033\Thermal=0.1358791\Dipole=-2.5014366,2.0690847,0.5824062\PG=C01 [X(C5H8Li1O2)]\\@

Mon Li+(O-methoxy,s-cis)

1\1\GINC-R140\FOpt\RM062X\6-31+G(d,p)\C5H8Li1O2(1+)\ROOT\22-Oct-2013\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=268435456\\MMA_mono_Li+.O-CH3.s-cis.1.freq\\1,1\C,0.0714301099,0.0377076971,-0.0640301013\O,-0.0215840552,-0.0170390117,1.3891496372\C,1.2223774474,-0.0964676842,2.0268832476\O,2.2246530782,-0.1137725125,1.3807662666\C,1.1041273629,-0.1509832581,3.5089984127\C,2.2473561909,-0.22819231,4.1958673948\H,3.1994743828,-0.2486001819,3.6751297764\H,2.2533669696,-0.2720958461,5.2801542611\C,-0.2526118021,-0.1184479135,4.165346793\H,-0.1548183376,-0.1657675904,5.2506871244\H,-0.7856732992,0.8283126716,3.9736558765\H,-0.8646146181,-0.9975994749,3.9011489088\H,-0.9517893925,0.0958595692,-0.4345773508\H,0.5650163437,-0.8629352015,-0.425830132\H,0.6402899919,0.9198182137,-0.3538235324\Li,-1.6343152493,0.0172339583,2.2623116874\\Version=ES64L-G09RevD.01\State=1-A\HF=-352.9829645\RMSD=9.703e-09\RMSF=5.327e-06\Dipole=-3.5074431,0.1324474,0.4672694\Quadrupole=7.8433205,-10.0321691,2.1888486,-0.9525575,4.4394655,-0.6868392\PG=C01 [X(C5H8Li1O2)]\\@

Mon Li+(O,O' bis,s-trans)

1\1\GINC-R113\FOpt\RM062X\6-31+G(d,p)\C5H8Li1O2(1+)\ROOT\22-Oct-2013\0\\#M062X/6-31+G(d,p) INT (gri
d=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=268435456\\MMA_mono_Li+.chelate.s-trans.freq\\1,1\C,0.09
25047342,-0.1975967231,0.0409081595\O,0.0334830508,0.2195587283,1.4300407414\C,1.0634467104,0.162268162
3,2.3072165709\O,0.7094812061,0.2682745691,3.4778536307\C,2.4790013075,0.0081807002,1.9103811844\C,2.93
44209055,0.6178884135,0.8097689141\H,2.2978849556,1.1855140781,0.1396185504\H,3.9938367442,0.597574508
7,0.5742446081\C,3.3408312214,-0.7083516287,2.9143734961\H,4.3723414528,-0.7421641552,2.5631696027\H,3.3
091004926,-0.1932758288,3.8777461446\H,2.9923491149,-1.7324095616,3.0749930154\H,-0.8707991046,-0.65839
74422,-0.1682824309\H,0.8985679894,-0.9154509606,-0.1009999313\H,0.2320863723,0.6808975462,-0.587687992\
Li,-1.1191996448,0.494983655,3.1994481921\\Version=ES64L-G09RevD.01\State=1-A\HF=-352.9968124\RMSD=9
.391e-09\RMSF=1.540e-05\Dipole=-2.5902686,0.2945515,0.0117393\Quadrupole=12.8903102,-9.6398226,-3.250487
6,-2.6639044,-6.5102736,0.3477714\PG=C01 [X(C5H8Li1O2),(X(H4)]\\@

Mon Li+(O,O' bis,s-cis)

1\1\GINC-R138\FOpt\RM062X\6-31+G(d,p)\C5H8Li1O2(1+)\ROOT\22-Oct-2013\0\\#M062X/6-31+G(d,p) INT(grid
=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=268435456\\MMA_mono_Li+.chelate.s-cis.freq\\1,1\C,0.07299
11256,-0.2685618567,0.0735577937\O,0.0208046548,0.2633688779,1.4218304493\C,1.0646341679,0.2081657395,2.
2864223355\O,0.7271529,0.3702289417,3.4561171357\C,2.4575824287,0.0059608433,1.8362261664\C,3.24954535
11,-0.6126240923,2.7227304144\H,2.8697794625,-0.9559216451,3.6794084131\H,4.2971633911,-0.7890291738,2.4
989975784\C,2.9424467984,0.5476544387,0.5117991137\H,-0.9548330759,-0.5204588559,-0.1783297002\H,0.6924
308579,-1.1655621835,0.0553280873\H,0.452173183,0.4924954976,-0.606014052\Li,-1.097713137,0.6237446571,3.
1659345925\H,4.0172299511,0.7220568143,0.5793172973\H,2.7733416674,-0.1433981187,-0.3173873495\H,2.4699
857601,1.5031739341,0.2679781364\\Version=ES64L-G09RevD.01\State=1-A\HF=-352.9963602\RMSD=7.051e-09\
RMSF=1.297e-05\Dipole=-2.4213386,0.1632781,0.2872409\Quadrupole=12.8576961,-9.5383277,-3.3193684,-3.8120
538,-6.4383866,0.8883392\PG=C01 [X(C5H8Li1O2)]\\@

Ester Binding Selectivity

Rad

1\1\GINC-V1258\Freq\UM062X\6-31+G(d,p)\C5H9O2(2)\BXN501\12-Jul-2012\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) SCF=tight Freq=(noraman) maxdisk=268435456\\MMA_rad.M062X.freq\\0,2\C,0.0047945073,0.,-0.0362715686\O,-0.0062279356,0.,1.3890906909\C,1.2191806355,0.,1.9675611915\O,2.2472533711,0.,1.3092365928\C,1.1695722399,0.,3.4208935312\C,2.4564530316,0.,4.1698763105\H,3.3080124942,0.,3.4892915192\H,2.5198599128,0.8791105831,4.8243771266\H,2.5198599128,-0.8791105831,4.8243771266\H,-1.0408710612,0.,-0.3398039738\H,0.516478661,-0.8882322002,-0.4137731502\H,0.516478661,0.8882322002,-0.4137731502\C,-0.1129681851,0.,4.1799224268\H,-0.98173758,0.,3.5232463818\H,-0.1649803325,0.8783464489,4.8368149722\H,-0.1649803325,-0.8783464489,4.8368149722\\Version=EM64L-G09RevA.02\State=2-A"\HF=-346.2267798\S2=0.758441\S2-1=0.\S2A=0.750049\RMSD=3.284e-09\RMSF=1.004e-04\ZeroPoint=0.1340553\Thermal=0.1431108\Dipole=-0.6760366,0.,0.5059796\PG=CS [SG(C5H3O2)]\\@

Mon

1\1\GINC-V1373\Freq\RM062X\6-31+G(d,p)\C5H8O2\BXN501\10-Jul-2012\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) SCF=tight Freq=(noraman) maxdisk=268435456\\MMA.a.M062X.freq\\0,1\C,-0.0404335614,0.,-0.123106065\O,0.0337832672,0.,1.3028467532\C,1.2783193205,0.,1.8088113138\O,2.2702054537,0.,1.1141723696\C,1.3229287015,0.,3.3033846124\C,0.1971402252,0.,4.0211239225\H,-0.7762970054,0.,3.544306561\H,0.232742561,0.,5.1065256993\C,2.7058582071,0.,3.8876343073\H,2.6614244396,0.,4.9782753493\H,3.2657787588,-0.8772332683,3.5515045882\H,3.2657787588,0.8772332683,3.5515045882\H,-1.1021744109,0.,-0.362853584\H,0.4475571379,-0.8890227765,-0.5279907051\H,0.4475571379,0.8890227765,-0.5279907051\\Version=EM64L-G09RevA.02\State=1-A'\HF=-345.6504672\RMSD=6.061e-09\RMSF=7.295e-05\ZeroPoint=0.1247988\Thermal=0.1327678\Dipole=-0.6480922,0.,0.2436116\PG=CS [SG(C5H4O2),X(H4)]\\@

Chain

1\1\GINC-V1312\Freq\RM062X\6-31+G(d,p)\C6H12O2\BXN501\11-Dec-2012\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) SCF=tight Freq=(noraman) maxdisk=268435456\\MMA_chain.1.freq\\0,1\C,0.1480191964,-0.3386418619,0.011466089\O,0.2788716159,-0.5008796937,1.4245360669\C,1.0902467171,0.3844996074,2.0340255507\O,1.6688728827,1.2568170321,1.4295810162\C,1.1716226766,0.1397221008,3.5362011884\H,-0.5329455178,-1.1228577557,-0.3144112774\H,-0.2586901497,0.6479657682,-0.220570128\H,1.1205263852,-0.444351715,-0.4737579769\C,1.7136050698,-1.2783839956,3.7768097376\C,2.1064566079,1.1789269373,4.1544277351\C,-0.2389230505,0.2655576115,4.1338982241\H,-0.188430446,0.1114914855,5.2166019732\H,-0.6558028078,1.2614964927,3.952367366\H,-0.9154627477,-0.4785920003,3.7067998319\H,1.7946076102,-1.4571366771,4.8538548502\H,1.0494110229,-2.0320851074,3.3470963856\H,2.7091305004,-1.3989484062,3.3374544797\H,2.1729869246,1.0129363265,5.2342043541\H,3.1097330653,1.1095717055,3.726082043\H,1.7392815489,2.1931132662,3.9770677245\\Version=EM64L-G09RevA.02\State=1-A\HF=-386.1743579\RMSD=2.685e-09\RMSF=1.367e-05\ZeroPoint=0.1761721\Thermal=0.1860555\Dipole=-0.4267931,-0.5709019,0.1344425\PG=C01 [X(C6H12O2)]\@

Rad-H

1\1\GINC-V1490\Freq\RM062X\6-31+G(d,p)\C5H10O2\BXN501\14-May-2013\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) SCF=tight Freq=(noraman) maxdisk=268435456\\MMA_rad_H.1.freq\\0,1\C,0.0175894852,0.1369437008,-0.0097369884\O,0.2418481204,0.4647826036,1.3625719438\C,0.9959138583,-0.4140676339,2.0492688734\O,1.462158848,-1.4091464381,1.5464822734\C,1.1471546944,-0.0017819854,3.4997386682\C,2.2261605543,-0.8345509943,4.1826406821\H,3.1874894138,-0.7385511081,3.6725315979\H,2.3462729994,-0.5114476903,5.2203663856\H,1.9518455073,-1.8929482951,4.175216921\H,-0.5989208775,0.9404303621,-0.4086147581\H,-0.4973381636,-0.8226664324,-0.0909615118\H,0.967610599,0.0763135291,-0.5447623828\C,-0.210407379,-0.1329028543,4.206720443\H,-0.972121414,0.4821060921,3.7226272007\H,-0.1176580381,0.1832659352,5.2493349535\H,-0.5443981881,-1.1757033418,4.1983575537\H,1.4311170006,1.0574905466,3.4960659116\\Version=EM64L-G09RevA.02\State=1-A\HF=-346.8762207\RMSD=3.001e-09\RMSF=3.875e-06\ZeroPoint=0.1482778\Thermal=0.1568422\Dipole=-0.3833387,0.5929753,0.1087559\PG=C01 [X(C5H10O2)]\\@

Rad Li+

1\1\GINC-V1383\Freq\UM062X\6-31+G(d,p)\C5H9Li1O2(1+,2)\BXN501\12-Jul-2012\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) SCF=tight Freq=(noraman) maxdisk=268435456\\MMA_rad_Li+.M062X.freq\\1,2\C,0.0055116527,0.,0.02265265\O,0.0072317085,0.,1.4570028304\C,1.1684941825,0.,2.0851534613\O,2.251723816,0.,1.4516061668\C,1.060131334,0.,3.5199823221\C,2.2810030362,0.,4.3652190677\H,3.2009375884,0.,3.7816352231\H,2.2789500348,0.8773635099,5.023568995\H,2.2789500348,-0.8773635099,5.023568995\H,-1.0432326165,0.,-0.2628082395\H,0.50

22211578,-0.8972133565,-0.3512219534\H,0.5022211578,0.8972133565,-0.3512219534\C,-0.2895698763,0.,4.14962
58475\H,-0.2101898576,0.,5.2370181224\H,-0.8683545541,0.8761093326,3.8353841715\H,-0.8683545541,-0.87610
93326,3.8353841715\Li,3.8021761074,0.,0.702143115\\Version=EM64L-G09RevA.02\State=2-A''\HF=-353.5887285
\S2=0.754811\S2-1=0.\S2A=0.750019\RMSD=3.392e-09\RMSF=5.770e-06\ZeroPoint=0.1364676\Thermal=0.147004
4\Dipole=2.9705656,0.,-1.7470108\PG=CS [SG(C5H3Li1O2),X(H6)]\\@

Mon Li+

1\1\GINC-V1483\Freq\RM062X\6-31+G(d,p)\C5H8Li1O2(1+)\BXN501\11-Dec-2012\0\\#M062X/6-31+G(d,p) INT(
grid=ultrafine) SCF=tight Freq=(noraman) maxdisk=268435456\\MMA_mono_Li+.freq\\1,1\C,-0.0106651276,0.,-0.0
245638821\O,0.0267947513,0.,1.419256883\C,1.1907636375,0.,2.0026318334\O,2.2498768662,0.,1.3506088875\C,1
.1853589852,0.,3.4837958155\C,0.0248683809,0.,4.1479397458\H,-0.925051572,0.,3.6248149863\H,0.0053717026,0
.,5.2331034087\C,2.5400414102,0.,4.1393280454\H,2.4449055439,0.,5.2255722271\H,3.1129013702,-0.8986068948,
3.8726835657\H,3.1129013702,0.8986068948,3.8726835657\H,-1.0668571012,0.,-0.2786453868\H,0.4826945735,-0.
8956739282,-0.4025648654\H,0.4826945735,0.8956739282,-0.4025648654\Li,3.9927010079,0.,1.6305373655\\Versi
on=EM64L-G09RevA.02\State=1-A'\HF=-353.0073407\RMSD=7.674e-09\RMSF=1.275e-05\ZeroPoint=0.1269835\
Thermal=0.1364259\Dipole=2.8976212,0.,-0.4728603\PG=CS [SG(C5H4Li1O2),X(H4)]\\@

Chain Li+

1\1\GINC-V1254\Freq\RM062X\6-31+G(d,p)\C6H12Li1O2(1+)\BXN501\13-Jul-2012\0\\#M062X/6-31+G(d,p) INT(
grid=ultrafine) SCF=tight Freq=(noraman) maxdisk=268435456\\MMA_sidechain_Li+.2.M062X.freq\\1,1\C,-0.06166
25293,0.,-0.0119012853\O,-0.0226838318,0.,1.4336378833\C,1.1399808547,0.,2.0172969094\O,2.1960179181,0.,1.3
66932996\C,1.0787339142,0.,3.5344022763\H,-1.1179165911,0.,-0.2655933171\H,0.4328515367,0.8950877275,-0.3
894644257\H,0.4328515367,-0.8950877275,-0.3894644257\C,0.3257609008,-1.2624485731,3.9929890225\C,0.3257
609008,1.2624485731,3.9929890225\C,2.5021129041,0.,4.1014432753\H,2.4691120208,0.,5.193219915\H,3.053209
9952,-0.9099721416,3.8189445247\H,3.0532099952,0.9099721416,3.8189445247\H,0.2820526588,-1.2759181753,5.
085208913\H,-0.6952277438,-1.265567978,3.6069749436\H,0.828115302,-2.1762843795,3.6602157568\H,0.282052
6588,1.2759181753,5.085208913\H,0.828115302,2.1762843795,3.6602157568\H,-0.6952277438,1.265567978,3.606
9749436\Li,3.8917992139,0.,1.9123021909\\Version=EM64L-G09RevA.02\State=1-A'\HF=-393.533889\RMSD=3.4
21e-09\RMSF=7.909e-06\ZeroPoint=0.1787044\Thermal=0.1898179\Dipole=2.9107573,0.,-0.5814182\PG=CS [SG(C
4H2Li1O2),X(C2H10)]\\@

Rad-H Li+

1\1\GINC-V1417\FOpt\RM062X\6-31+G(d,p)\C5H10Li1O2(1+)\BXN501\14-May-2013\0\\#M062X/6-31+G(d,p) IN
T(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=268435456\\MMA_rad_H_Li+.1.freq\\1,1\C,-0.2804375
833,-0.0287082165,-0.0360784248\O,-0.1174143827,-0.0515948959,1.4010602694\C,1.087606503,0.0114894076,1.8
843101018\O,2.0862786185,0.0901155656,1.1536365812\C,1.1536572301,-0.0352954011,3.3926675583\C,2.584911
0193,0.1708525543,3.8842679965\H,3.0050529661,1.1285213171,3.5473794554\H,2.6121604526,0.1947064462,4.9
751875639\H,3.2283560021,-0.671305004,3.5874482203\H,-1.3524720895,-0.0930568495,-0.1989493446\H,0.2356
94781,-0.8829667214,-0.4742850215\H,0.1214391135,0.9036904289,-0.4328521216\C,0.5558813956,-1.3587848221
,3.9008507951\H,-0.4785063915,-1.4724233627,3.5741300272\H,0.5771730769,-1.3718464146,4.9923706691\H,1.1
348836768,-2.2140347911,3.5384972189\H,0.5220602698,0.7871076439,3.7496012768\Li,3.8220970941,0.2399284
441,1.5201111736\\Version=EM64L-G09RevA.02\State=1-A\HF=-354.2342463\RMSD=8.236e-09\RMSF=2.970e-0
5\Dipole=2.7923291,0.4839386,-0.5667177\Quadrupole=11.2812456,-9.4426584,-1.8385872,3.0679584,-0.3458887,-
0.9500607\PG=C01 [X(C5H10Li1O2)]\\@

Rad Li+(Mon)

1\1\GINC-V1489\Freq\UM062X\6-31+G(d,p)\C10H17Li1O4(1+,2)\BXN501\21-Feb-2013\0\\#M062X/6-31+G(d,p) I
NT(grid=ultrafine) SCF=tight Freq=(noraman) maxdisk=268435456\\MMA_rad_mono_Li+.2.freq\\1,2\C,2.27338831
08,2.3821653844,0.4014719019\O,3.2268194413,1.3330562488,0.2018816967\C,2.7625066497,0.1003567277,0.041
983123\O,1.53938789,-0.1399615056,0.061173555\C,3.7920910049,-0.8894997251,-0.1490646314\C,5.2219289761,
-0.470759333,-0.1509276116\C,3.4253605908,-2.3158962037,-0.3423841492\H,3.8943497175,-2.931701636,0.4349
119146\H,2.348350341,-2.4783643083,-0.3196474845\H,3.8192906824,-2.6773458908,-1.3002583101\H,2.8610667
681,3.2911234318,0.5036041527\H,1.6961602841,2.1964838775,1.3096966194\H,1.6067168807,2.4526225483,-0.4
607112934\Li,-0.1676407475,-0.5833019354,0.0815411478\O,-1.9486936423,-0.8548038584,0.0881164571\C,-3.048
1748327,-0.2948371785,0.0074930282\O,-4.1704382741,-0.9659402985,0.0738692832\C,-4.0852295585,-2.3934636
055,0.2456725365\H,-5.1153760559,-2.7379898083,0.2747359309\H,-3.5503942159,-2.8342429475,-0.5963057608\
H,-3.5712153297,-2.621856317,1.1799539359\C,-3.181150279,1.1725339632,-0.1697658229\C,-1.8887791323,1.937

8412577,-0.2479570675\H,-2.0840258602,3.0033219875,-0.3747595648\H,-1.2989290139,1.8142179585,0.6682138273\H,-1.2829089648,1.6069340294,-1.0998210215\C,-4.3949352444,1.7267980311,-0.2489533501\H,-4.5073937962,2.7985203442,-0.3783805467\H,-5.2960456778,1.1271054317,-0.1869371986\H,5.8768820855,-1.3291976796,-0.3038347132\H,5.4138562482,0.2664432378,-0.9389448682\H,5.489748754,0.0160727716,0.7937522844\\Version=EM64L-G09RevA.02\State=2-A\HF=-699.297461\S2=0.75525\S2-1=0.\S2A=0.750022\RMSD=3.544e-09\RMSF=3.295e-06\ZeroPoint=0.2628186\Thermal=0.2831234\Dipole=-0.1327061,-0.2573536,0.0342417\PG=C01 [X(C10H17Li1O4)]\\@

Mono Li+(Mon)

1\1\GINC-V1258\Freq\RM062X\6-31+G(d,p)\C10H16Li1O4(1+)\BXN501\19-Jul-2012\0\\#M062X/6-31+G(d,p) INT (grid=ultrafine) SCF=tight Freq=(noraman) maxdisk=268435456\\Li+_MMA2.a.freq\\1,1\C,-0.3482980191,-0.0245484496,-0.3076501451\O,-0.3520365027,-0.0180329741,1.1321153991\C,0.8059142234,-0.0148343234,1.7434275163\O,1.8722312538,-0.0167242254,1.1158141145\C,0.7551097968,-0.0091374226,3.225957396\C,-0.4270314159,-0.0083332388,3.8503649151\H,-1.3598304482,-0.0116411877,3.2978175238\H,-0.4801817782,-0.0043304258,4.9343657748\C,2.0865938401,-0.0047382245,3.9249467372\H,1.9489865832,-0.0012989972,5.0066711533\H,2.6728740589,-0.8952997108,3.6700592845\H,2.6700769796,0.8859651724,3.6641051495\H,-1.3963807775,-0.0265876733,-0.5945075341\H,0.156674082,-0.9204038766,-0.6706124425\H,0.1551943292,0.8688704328,-0.6788211715\Li,3.6649116876,-0.0101718155,1.2710760587\O,5.4575719031,-0.0030247363,1.4273836654\C,6.5236805419,-0.0028718756,0.7994074559\O,7.6818282691,0.004312104,1.4102930242\C,7.6785478054,0.0120523255,2.8500593257\H,8.7267240601,0.017215297,3.136565919\H,7.1714073819,0.9069589412,3.2124875276\H,7.1775897385,-0.8823867184,3.222113774\C,6.5739836276,-0.0106379465,-0.683140358\C,5.2422637902,-0.0190021174,-1.3816454488\H,5.3794830786,-0.0243676804,-2.4634117162\H,4.6605454761,-0.910268834,-1.118813521\H,4.6544170925,0.8710207743,-1.1284127113\C,7.7558967438,-0.0099096484,-1.3079748356\H,7.8086826871,-0.0155183173,-2.3919870336\H,8.6888806147,-0.0036952754,-0.7557639434\\Version=EM64L-G09RevA.02\State=1-A\HF=-698.7169054\RMSD=6.988e-09\RMSF=9.238e-06\ZeroPoint=0.2533226\Thermal=0.2726569\Dipole=0.0003675,0.0003974,-0.0009088\PG=C01 [X(C10H16Li1O4)]\\@

Chain Li+(Mon)

1\1\GINC-V1490\Freq\RM062X\6-31+G(d,p)\C11H20Li1O4(1+)\BXN501\21-Feb-2013\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) SCF=tight Freq=(noraman) maxdisk=268435456\\MMA_chain_mono_Li+.2.freq\\1,1\C,2.9756170352,2.8911552917,0.5558168971\O,3.406043478,1.5210261785,0.4324459157\C,2.4875133472,0.6057143144,0.2563549797\O,1.2888867289,0.8961101578,0.1964770936\C,3.0395981068,-0.8039654027,0.1379677062\C,3.9978805264,-0.8509706222,-1.0660204429\C,3.8034369351,-1.1368675692,1.4325188706\H,4.1990838478,-2.1536348749,1.3614557255\H,4.6393318203,-0.4503860593,1.5803455254\H,3.1496879706,-1.0871055638,2.3090498854\H,3.8880137678,3.4652682201,0.6924466148\H,2.3170507838,2.9930985401,1.4189597105\H,2.4547395737,3.1958536185,-0.3524586654\Li,-0.2527085477,-0.0338050892,-0.0298897462\O,-1.9065340362,-0.7176646403,-0.236895468\C,-3.1071884034,-0.4257895989,-0.2967668363\O,-4.0290894933,-1.3391408349,-0.4735133718\C,-3.5986085753,-2.7074233163,-0.5972043681\H,-4.5111961545,-3.2811954434,-0.7342372507\H,-2.9405905638,-2.8100909955,-1.4608418498\H,-3.0786556346,-3.0137150532,0.3112190832\C,-3.5943383815,0.9701759135,-0.1742839959\C,-2.5332922147,2.0163436543,0.0285075273\H,-2.9846007831,3.0059092496,0.1071471575\H,-1.9677590048,1.8373437443,0.9503556145\H,-1.8306317343,2.0399866349,-0.8125549518\C,-4.9046331144,1.2253941999,-0.2469465908\H,-5.2760628306,2.2413851552,-0.1591154058\H,-5.6291831832,0.4324814522,-0.3944086275\H,4.3958209437,-1.8644601027,-1.1654556588\H,3.4848863812,-0.5943320635,-1.9982979118\H,4.8343808871,-0.1634817051,-0.9265287879\C,1.8860072086,-1.7889585444,-0.0645151249\H,1.1980419087,-1.7912046484,0.7907438831\H,1.3368076469,-1.5870023978,-0.9931504741\H,2.2815962191,-2.803812969,-0.1499136861\\Version=EM64L-G09RevA.02\State=1-A\HF=-739.2424829\RMSD=2.811e-09\RMSF=2.019e-06\ZeroPoint=0.3049504\Thermal=0.3260617\Dipole=-0.4830728,0.0748427,-0.0290556\PG=C01 [X(C11H20Li1O4)]\\@

Rad-H Li+(Mon)

1\1\GINC-V1347\FOpt\RM062X\6-31+G(d,p)\C10H18Li1O4(1+)\BXN501\10-Sep-2013\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=268435456\\MMA_rad_H_mono_Li+.2.freq\\1,1\C,-0.0245335126,0.0742388308,0.0205532233\O,-0.0122778617,0.0403992349,1.4619795039\C,1.1490149245,-0.0025833811,2.0618773047\O,2.2094154054,-0.0125734851,1.4302610031\C,1.051457096,-0.0533550728,3.5683049803\H,0.4357216707,0.806414412,3.8587240791\C,0.3169173381,-1.3361522276,3.9945867381\H,0.2190905884,-1.3535104642,5.0820652757\H,-0.6809573974,-1.3845751657,3.5564647565\H,0.8788013635,-2.2249534383,3.6904882746\H,-1.0752358789,0.1055692086,-0.2544482944\H,0.455747899,-0.8226235027,-0.3718742973\H,0.4974773957,0.9650982931,-0.330122472\Li,3.9805448325,-0.0067045324,1.8184266572\O,5.7704580844,-0.0008374086,2.0130186471\C,6.8420540921,-0.0059580587,1.3945529583\O,7.9947376999,0.0042892946,2.0158467804\C,7.977788276,0.0224

144286,3.4554302104\H,9.0232011935,0.0279883338,3.7518876118\H,7.468559599,0.9206251759,3.8065488694\H,
7.4716393209,-0.8683723417,3.8291736425\C,6.9054354618,-0.0237943375,-0.0875245543\C,5.5796875249,-0.033
9041289,-0.7973368963\H,5.7261555168,-0.0462399633,-1.8778412526\H,4.9931582145,-0.9218792686,-0.5340372
745\H,4.990865974,0.8583992886,-0.5546327854\C,8.0927486023,-0.0297324011,-0.701963591\H,8.1549783448,-0.
0426992869,-1.7854346713\H,9.0209222652,-0.0217059106,-0.1417218256\C,2.4294755329,0.0575757619,4.21422
37777\H,3.0473371254,-0.8180520947,3.9766144579\H,2.9520009074,0.9742624213,3.9180837835\H,2.330611484
3,0.0838324478,5.3011809942\\Version=ES64L-G09RevD.01\State=1-A\HF=-699.943406\RMSD=7.718e-09\RMSF
=2.356e-06\Dipole=0.0989577,0.099574,-0.0383273\Quadrupole=18.8552623,-18.6471836,-0.2080787,0.7569607,-1.
8326108,-0.5527294\PG=C01 [X(C10H18Li1O4)]\\@

Rad Li+(Mon)$_2$

1\1\GINC-V1264\Freq\UM062X\6-31+G(d,p)\C15H25Li1O6(1+,2)\BXN501\07-Mar-2013\0\\#M062X/6-31+G(d,p) I
NT(grid=ultrafine) SCF=tight Freq=(noraman) maxdisk=671088640\\MMA_rad_Li+.MMA2.freq\\1,2\Li,0.30851565
86,-0.0069876918,-0.1183998869\O,-0.3323567725,-1.6847129012,-0.6099597779\O,1.9369559845,0.0136392376,0.
7759332244\O,-0.6732354825,1.5065329037,-0.3820246\C,-1.6558716716,2.2644342429,-0.3850915324\C,3.110425
9234,0.1357937633,0.4259463314\C,-1.0857597362,-2.5223976151,-0.1147850726\C,-1.6986439671,-2.3539728247,
1.2301822835\O,-1.4090163293,-3.6301770238,-0.7479647494\C,-0.8411832581,-3.8245808577,-2.0543574466\H,-1
.2283978474,-4.7810754988,-2.3957931445\H,-1.1540312437,-3.0177570411,-2.718772833\H,0.2472080789,-3.8479
899922,-1.9849115709\C,-1.2598764309,-1.1340543053,1.9924137864\H,-1.7282248102,-1.1101260208,2.97721379
07\H,-0.1729027623,-1.1246574133,2.1328736173\H,-1.5422877641,-0.2137778879,1.4654658519\C,-2.5739291425
,-3.2566011568,1.683530315\H,-3.0281038077,-3.1441782829,2.6630566774\H,-2.8514196795,-4.1220921605,1.092
4589227\O,-1.5128310973,3.5821922046,-0.281685715\C,-3.0296390519,1.8288344318,-0.4973781203\C,-0.175123
4104,4.0815313013,-0.1635762028\H,-0.2762760954,5.1603540337,-0.0735711763\H,0.3056074961,3.6617509069,0
.722041356\H,0.4008014689,3.8221610808,-1.0540616042\C,-3.3229536051,0.3876933448,-0.7255366656\H,-4.047
6326385,0.277230712,-1.5401753207\H,-2.4230076677,-0.1799701097,-0.9680814117\H,-3.7905903649,-0.0552859
948,0.1653658544\C,-4.1457449304,2.8129439354,-0.4374024082\H,-4.3294179031,3.2355613325,-1.4354377638\H
,-3.920845107,3.649534131,0.2259767265\O,4.1027785576,0.1050864237,1.2906077604\C,3.7577138874,-0.081136
3018,2.6729493337\H,4.7034449383,-0.0711670773,3.2086613825\H,3.1119721405,0.7321197693,3.0071722558\H,
3.2482724415,-1.0372527384,2.8019731551\C,3.5067357919,0.3279144694,-0.9943114066\C,2.371735579,0.346577
3706,-1.9810592106\H,2.7481409062,0.4921906876,-2.9942740534\H,1.8176462869,-0.5998892007,-1.9641609088\
H,1.6719460511,1.1632049613,-1.7649083014\C,4.7954051022,0.4683735794,-1.317737677\H,5.5734397979,0.445
4974608,-0.5631108608\H,5.0949120837,0.6093058474,-2.3514702664\H,-5.0693120574,2.3257615514,-0.1159183
452\\Version=EM64L-G09RevA.02\State=2-A\HF=-1044.9883582\S2=0.755802\S2-1=0.\S2A=0.750027\RMSD=3.2
59e-09\RMSF=3.955e-06\ZeroPoint=0.3898086\Thermal=0.4192956\Dipole=-0.063612,-0.0730029,0.
0021775\PG=C01 [X(C15H25Li1O6)]\\@

Mon Li+(Mon)$_2$

1\1\GINC-V1294\Freq\RM062X\6-31+G(d,p)\C15H24Li1O6(1+)\BXN501\22-Feb-2013\0\\#M062X/6-31+G(d,p) IN
T(grid=ultrafine) SCF=tight Freq=(noraman) maxdisk=671088640\\MMA_mono_Li+.MMA2.freq\\1,1\Li,0.51794845
84,-0.6405483295,0.6819098325\O,-0.0324992057,-0.4304910488,2.4390692302\O,2.0620592553,0.2650041723,0.2
294838124\O,-0.1273088981,-1.9496511614,-0.4446149084\C,-0.5508425253,-3.0716395479,-0.7218692553\C,3.27
44047488,0.1540233989,0.4043446058\C,-1.0280348611,-0.1769493529,3.116508748\C,-2.3033581499,0.30040260
86,2.5220929033\O,-1.0306259756,-0.3199841978,4.4257422927\C,0.1830939532,-0.7929796614,5.0309887066\H,-
0.0230154024,-0.8311909823,6.0975459383\H,0.4256682608,-1.7861290911,4.647671446\H,0.9994142053,-0.10151
85726,4.816617889\C,-2.2873949567,0.4974081611,1.0317107971\H,-3.2553300848,0.8604099583,0.6843068324\H
,-1.5271914424,1.2310476747,0.740145054\H,-2.070940998,-0.4420633631,0.5098616697\C,-3.3636064704,0.52172
46758,3.3054402308\H,-4.3008304289,0.8693976152,2.8825270689\H,-3.3187348009,0.3641791445,4.3771412329\
O,-0.6157534561,-3.5005475424,-1.9646872114\C,-1.0228089954,-4.032800831,0.3085655126\C,-0.1589981323,-2.
6057889797,-2.9923799889\H,-0.2900795952,-3.1494213716,-3.9244030533\H,-0.7602783988,-1.6956121274,-2.98
54042498\H,0.8910974249,-2.3584966736,-2.8299271297\C,-1.0513174612,-3.513396755,1.7184752175\H,-1.38001
20157,-4.2961835725,2.4033496497\H,-0.0622197981,-3.1633921093,2.0331418292\H,-1.7395010715,-2.665018277
1,1.8070088941\C,-1.3856805946,-5.2679970867,-0.0515120584\H,-1.7273908603,-5.9821335837,0.6910627867\H,-
1.3497247761,-5.5908663087,-1.0857638116\O,4.1258537686,1.0639942937,-0.0199226973\C,3.576164475,2.20648
20792,-0.6970871459\H,4.4319785427,2.8227626917,-0.9602073182\H,3.0382006523,1.8849721967,-1.5898867967\
H,2.9004891842,2.7429637491,-0.0295840877\C,3.8827305327,-1.0098210962,1.1030607515\C,2.9113723565,-2.04
91832719,1.5911970554\H,3.4421756175,-2.8681536123,2.0786487926\H,2.2055342281,-1.6196358063,2.31225891
81\H,2.3347313232,-2.469284446,0.7580772096\C,5.2078093029,-1.5898867967\H,2.9004891842,2.7429637491,-0.
0295840877\C,3.8827305327,-1.0098210962,1.1030607515\C,2.9113723565,-2.0491832719,1.5911970554\H,3.4421
756175,-2.8681536123,2.0786487926\H,2.2055342281,-1.6196358063,2.3122589181\H,2.3347313232,-2.469284446,

0.7580772096\C,5.2078093029,-1.0788311904,1.2595434666\H,5.8625776388,-0.2987418423,0.8881050484\H,5.66
24876481,-1.9243985457,1.7660073576\\Version=EM64L-G09RevA.02\State=1-A\HF=-1044.4084956\RMSD=4.37
6e-09\RMSF=4.838e-06\ZeroPoint=0.3801975\Thermal=0.4088058\Dipole=0.0023615,0.0214126,-0.0806312\PG=C
01 [X(C15H24Li1O6)]\\@

Chain Li+(Mon)$_2$

1\1\GINC-V1463\Freq\RM062X\6-31+G(d,p)\C16H28Li1O6(1+)\BXN501\22-Feb-2013\0\\#M062X/6-31+G(d,p) IN
T(grid=ultrafine) SCF=tight Freq=(noraman) maxdisk=671088640\\MMA_chain_Li+.MMA2.freq\\1,1\Li,0.46812566
25,-0.6465544692,0.6800716663\O,-0.0772954552,-0.3943212992,2.431270543\O,2.0650198588,0.1710906982,0.23
44555101\O,-0.2575271597,-1.8991921363,-0.4633545996\C,-0.7817477895,-2.9721369928,-0.7516706055\C,3.266
9426561,-0.0151445266,0.4160895602\C,-1.0709160479,-0.1469788227,3.1133023582\C,-2.3346492908,0.37656827
,2.5325327808\O,-1.0825029275,-0.337067399,4.4165988713\C,0.1165758071,-0.8622270867,5.0074889361\H,-0.09
36076894,-0.9321706564,6.0716555232\H,0.3332998299,-1.847650087,4.5900693857\H,0.9515103263,-0.18565260
94,4.8190008224\C,-2.3126163069,0.6195202984,1.0491422413\H,-3.2704359803,1.0190595013,0.7138057702\H,-1
.5320664866,1.339781633,0.7798145708\H,-2.1207655755,-0.3093096354,0.4990582573\C,-3.3908250761,0.597341
7751,3.3214820569\H,-4.3191312092,0.979654202,2.9088772819\H,-3.3511833238,0.4056030515,4.3877669965\O,-
0.9393276756,-3.3449644957,-2.0044473456\C,-1.2788267179,-3.9991816403,0.2511037878\C,-0.4648289372,-2.45
15966762,-3.0263860455\H,-0.6852979217,-2.9484891169,-3.9676225713\H,-0.9900454543,-1.4979804176,-2.9580
235933\H,0.608390812,-2.2930970609,-2.9113950763\C,-0.3413546026,-5.2188299871,0.1617686768\H,-0.6707345
075,-5.9742557094,0.8807340044\H,-0.3628358879,-5.6602457734,-0.837210021\H,0.6913320253,-4.9474904381,0.
4055251598\C,-1.2379693962,-3.4025303685,1.6582725469\H,-1.8933605945,-2.5280603611,1.7380425035\H,-0.22
3909759,-3.1003384723,1.9399116624\O,4.1754034412,0.8479506246,0.012803567\C,3.7008929146,2.0324459578,
-0.649060149\H,4.5942748974,2.6004967927,-0.895277585\H,3.152332363,1.7583695984,-1.5511999468\H,3.05275
90841,2.5972678869,0.0223656768\C,3.7976949879,-1.2247738632,1.1003245832\C,2.7590952839,-2.2103736785,1
.5604638111\H,3.2324427881,-3.0731455032,2.0315530066\H,2.0779035511,-1.7525053786,2.2879913759\H,2.160
9631324,-2.5711530711,0.7145762926\C,5.1143485772,-1.3768290425,1.26811017\H,5.8187610892,-0.6315879886,
0.9164034661\H,5.5119367754,-2.2566543113,1.7641276349\H,-1.5839136443,-4.1511506826,2.37620678\C,-2.713
6967913,-4.4127747098,-0.1143129701\H,-3.0704682533,-5.1443318491,0.615962571\H,-3.3928190919,-3.5543392
079,-0.0929036158\H,-2.7554073718,-4.8647560247,-1.1069521652\\Version=EM64L-G09RevA.02\State=1-A\HF=-
1084.9334273\RMSD=6.430e-09\RMSF=4.531e-06\ZeroPoint=0.4317685\Thermal=0.4621828\Dipole=0.2184371,0.
3893982,-0.0416244\PG=C01 [X(C16H28Li1O6)]\\@

Rad-H Li+(Mon)$_2$

1\1\GINC-V1364\FOpt\RM062X\6-31+G(d,p)\C15H26Li1O6(1+)\BXN501\10-Sep-2013\0\\#M062X/6-31+G(d,p) IN
T(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=671088640\\MMA_rad_H_Li+.MMA2.freq\\1,1\Li,-0.05
43068772,-0.1281479075,0.0237423362\O,-0.0411591086,-0.1669828808,1.8767064133\O,1.6177730399,0.0312143
86,-0.7473340332\O,-1.5137217552,-0.4998916474,-1.0452792527\C,-2.6051117978,-0.9975391,-1.3077761456\C,2.
5763334694,-0.7028831578,-0.9818441353\C,-0.5454519632,0.4041940773,2.8427403075\C,-1.3260216832,1.66215
20835,2.7124861574\O,-0.4315498125,-0.0687611234,4.0663138447\C,0.3012401932,-1.2944411477,4.2234181018\
H,0.2787508031,-1.5085254446,5.2888339539\H,-0.1848714335,-2.091169265,3.6570048573\H,1.3264663696,-1.16
14822923,3.8746377201\C,-1.4233226325,2.2197621827,1.3195175743\H,-1.9893540925,3.1519992887,1.31967942
51\H,-0.429051304,2.428246864,0.9082307387\H,-1.9294548063,1.5176193141,0.64595694\C,-1.8848960803,2.217
0011532,3.7924103594\H,-2.4575230478,3.1353539885,3.7093503574\H,-1.7814018102,1.7714026851,4.775297950
4\O,-3.0861749732,-1.0064628554,-2.5327641364\C,-3.5322214485,-1.6415570245,-0.3034261638\C,-2.2842730306
,-0.4049703052,-3.564106453\H,-2.8578163797,-0.5235366178,-4.4796884498\H,-2.1226595091,0.6502019251,-3.3
396252434\H,-1.3254021121,-0.9203229573,-3.636194018\H,-3.7218060275,-2.6538275144,-0.6820064128\C,-2.891
0694167,-1.7130273186,1.0780468923\H,-2.7593371399,-0.7071963129,1.4917822187\H,-1.9131483427,-2.2034375
895,1.0531950949\O,3.6954328887,-0.243759992,-1.5013811246\C,3.754915593,1.1648447639,-1.7808031293\H,4.
7441669408,1.3325819313,-2.1988067373\H,2.9780743954,1.4338132508,-2.4977882165\H,3.6208950579,1.731329
6473,-0.8582488573\C,2.5560365127,-2.16409111,-0.7040121993\C,1.2794728062,-2.689073885,-0.1065097164\H,1
.3461486111,-3.7667531109,0.0487753874\H,1.0733948728,-2.2163970495,0.8612976187\H,0.4276592183,-2.49678
20406,-0.7703246623\C,3.6251890018,-2.9141952763,-0.9855328322\H,4.521770996,-2.4819819589,-1.4151991229
\H,3.6205094193,-3.9816576715,-0.7888368501\H,-3.5402845623,-2.2720700554,1.7556856385\C,-4.8700337815,-0
.8835027726,-0.2763115015\H,-5.5470165499,-1.367307157,0.4312150915\H,-4.7205632632,0.1501396899,0.05314
98363\H,-5.3435872331,-0.8734585312,-1.2590551688\\Version=ES64L-G09RevD.01\State=1-A\HF=-1045.6343957
\RMSD=4.890e-09\RMSF=3.135e-06\Dipole=0.168414,0.0559326,-0.0932066\Quadrupole=4.2373862,-7.4899789,3.
2525928,-2.7637696,-4.154184,0.2647244\PG=C01 [X(C15H26Li1O6)]\\@

Rad Li+(Mon)$_3$

1\1\GINC-V1420\Freq\UM062X\6-31+G(d,p)\C20H33Li1O8(1+,2)\BXN501\30-Dec-2012\0\\#M062X/6-31+G(d,p) I
NT(grid=ultrafine) SCF=tight Freq=(noraman) maxdisk=1342177280\\MMA_rad_Li+.MMA3.freq\\1,2\Li,-0.0063168
924,-0.0655219208,-0.0023469525\O,0.0038087769,-0.0517920377,1.9139300524\O,1.9012432909,0.0345072811,-0
.3074996202\O,-0.7441282423,-1.6953234629,-0.5178903589\O,-0.5997802068,1.4805921241,-0.9204320657\C,-0.2
972724972,2.6311889395,-1.2125591786\C,-0.5401384505,-2.8954303711,-0.7320433475\C,2.9180920949,-0.12189
28786,0.3591698069\C,-0.7021939602,0.0856663035,2.9084074269\C,-2.176688062,0.267511029,2.8397009768\O,-
0.1888552233,0.0765052927,4.1279115266\C,1.2300183328,-0.1107142896,4.2224628066\H,1.4582027494,-0.0653
685955,5.2846300852\H,1.5080975644,-1.0811467491,3.8054467664\H,1.7509593332,0.6797897609,3.677995096\C
,-2.7606758339,0.3039831319,1.4555457086\H,-3.8448062483,0.4143422645,1.505471126\H,-2.3521904074,1.1398
603839,0.8776716953\H,-2.5238656301,-0.6103791875,0.9008323232\C,-2.8845267782,0.3825054366,3.968301145
3\H,-3.9616366781,0.5125434065,3.9326624604\H,-2.4098099578,0.3501209546,4.9423729695\O,-0.5000090878,3.
1246911309,-2.4220856014\C,0.3102298432,3.5848867169,-0.2422312202\C,0.4327023696,3.0831615701,1.168699
0177\H,0.8960122678,3.841349128,1.8024239418\H,-0.5521140602,2.8380019557,1.5817672282\H,1.0292571358,2
.1652639139,1.2128119843\C,0.7016379827,4.7960520385,-0.6507533752\H,1.1448957553,5.4987075025,0.048335
2127\H,0.5837494258,5.1119067407,-1.6810965975\C,-1.0787099403,2.2370129347,-3.3900038513\H,-1.177373533
2,2.8256656808,-4.2986922245\H,-0.4190779329,1.3822820525,-3.55001954\H,-2.0527384174,1.8901017828,-3.042
1741393\O,0.0961784231,-3.315789146,-1.8277291478\C,-0.9441011268,-3.9467035387,0.1747983517\C,0.5281992
708,-2.2959761385,-2.7354723294\H,1.0367984964,-2.8209537019,-3.5409305203\H,-0.3349152503,-1.7462867063,
-3.1169716934\H,1.207415343,-1.6043416451,-2.2294651761\C,-1.6083024029,-3.5495181539,1.447760717\H,-1.39
9303093,-4.2781922311,2.2357450408\H,-1.2918898114,-2.5540073811,1.7706830456\H,-2.6996333902,-3.5187511
687,1.3173591695\C,-0.740492419,-5.3867878027,-0.1396474307\H,0.0151502192,-5.8144494693,0.5334599716\H,
-0.4173162139,-5.5474328247,-1.1670608001\O,3.9081210118,0.7566792954,0.3440890927\C,3.7478226815,1.8993
287486,-0.5090706535\H,4.6732493276,2.4622585784,-0.413650956\H,3.5951724616,1.5752384178,-1.5398301805\
H,2.8955686571,2.4992400141,-0.1837020116\C,3.1586965825,-1.3105641635,1.2260073911\C,2.1571211975,-2.42
33839204,1.0997872856\H,2.4432593306,-3.2647068184,1.7343675195\H,1.1594723875,-2.0787625613,1.39056187
2\H,2.0982401476,-2.7766379006,0.0638978044\C,4.219206107,-1.3374580587,2.0394628344\H,4.919392604,-0.51
11516911,2.0871367695\H,4.4079588545,-2.1993363583,2.6725226932\H,-1.6656681945,-5.9459842375,0.0414501
468\\Version=EM64L-G09RevA.02\State=2-A\HF=-1390.6696023\S2=0.755824\S2-1=0.\S2A=0.750027\RMSD=8.0
25e-09\RMSF=5.350e-06\ZeroPoint=0.5159889\Thermal=0.5548644\Dipole=0.2701666,0.0664691,0.0722432\\PG=C
01 [X(C20H33Li1O8)]\\@

Mon Li+(Mon)$_3$

1\1\GINC-V1421\Freq\RM062X\6-31+G(d,p)\C20H32Li1O8(1+)\BXN501\30-Dec-2012\0\\#M062X/6-31+G(d,p) IN
T(grid=ultrafine) SCF=tight Freq=(noraman) maxdisk=1342177280\\MMA_mono_Li+.MMA3.freq\\1,1\Li,-0.102371
6156,-0.0940483167,-0.1784161736\O,-0.0599207691,-0.2750123807,1.7213394344\O,1.7861227021,-0.2112188803
,-0.5581487758\O,-0.999258189,-1.6225682022,-0.8292409\O,-0.5759721405,1.5517281126,-0.9596600367\C,-0.208
1191448,2.7057872437,-1.1454358809\C,-0.8743847501,-2.8062962469,-1.1213473818\C,2.8105576988,-0.4910597
499,0.055503223\C,-0.7698131904,-0.292594427,2.7228870095\C,-2.2292262777,-0.0088392999,2.6916010175\O,-0
.2751758051,-0.5751065477,3.9167935653\C,1.1275671954,-0.8689373226,3.9769542916\H,1.3437897197,-1.03443
24361,5.0296510555\H,1.3475804693,-1.7633059497,3.3897185683\H,1.7051668526,-0.028180377,3.5874299101\C
,-2.7887905945,0.3588642028,1.3467159202\H,-3.8630511174,0.5345807753,1.4188978969\H,-2.3138512594,1.264
8027147,0.9557899892\H,-2.6102877707,-0.4369429067,0.6157413101\C,-2.9467794786,-0.0969364878,3.81639212
5\H,-4.0137163294,0.1027845738,3.8067601544\H,-2.4902209139,-0.3675040314,4.7616711175\O,-0.4565389351,3
.3469858514,-2.2739628076\C,0.5360737288,3.49786494,-0.1263633167\C,0.6906845131,2.8448471532,1.21809810
87\H,1.2602332268,3.4897880099,1.8894689866\H,-0.287268021,2.6483455092,1.6707374152\H,1.1977163389,1.8
77069609,1.1375878159\C,1.0123275001,4.7073835347,-0.4385067727\H,1.5571384073,5.2931976871,0.295560999
2\H,0.865164699,5.1377641445,-1.422599735\C,-1.1692537316,2.6185540243,-3.2847801601\H,-1.284140172,3.312
743646,-4.1135105563\H,-0.5924070852,1.7429959439,-3.5877592271\H,-2.1412049909,2.3044069761,-2.90171206
17\O,-0.275456311,-3.2003917131,-2.2334449612\C,-1.3698531178,-3.8999596284,-0.2439361661\C,0.2292907846,
-2.163324625,-3.0881029145\H,0.6960236809,-2.6798250863,-3.9234404437\H,-0.5943004182,-1.5351827407,-3.43
28880919\H,0.9564454368,-1.5543269956,-2.5453467657\C,-2.0464692297,-3.4495115503,1.0197543726\H,-2.3346
705372,-4.3089139417,1.6264264245\H,-1.3807521401,-2.8094295448,1.6095527961\H,-2.9423520381,-2.86172816
47,0.7969236877\C,-1.1913475602,-5.1761158095,-0.5991520491\H,-1.543229262,-5.9817002319,0.0376936293\H,-
0.6991497332,-5.4419536144,-1.52793861\O,3.8706645718,0.300422788,0.0473796706\C,3.7771187847,1.5027709
85,-0.7306773939\H,4.7497913786,1.9804303216,-0.6407808498\H,3.5605527281,1.2559476678,-1.7713362948\H,2
.9912150464,2.1498774704,-0.3361140808\C,2.9774947386,-1.7453286922,0.8420997523\C,1.8910432309,-2.76865
90754,0.6716487271\H,2.1077684686,-3.659657937,1.2640837841\H,0.9252799306,-2.3589287836,0.984642799\H,
1.800972387,-3.0695841121,-0.3783106343\C,4.0479332577,-1.9012157801,1.6275511441\H,4.8099836336,-1.1341
692971,1.7073519012\H,4.182026695,-2.8114831947,2.2043581856\\Version=EM64L-G09RevA.02\State=1-A\HF=-

1390.0905974\RMSD=7.200e-09\RMSF=2.848e-06\ZeroPoint=0.5066408\Thermal=0.5444665\Dipole=0.4192211,0.1910224,-0.0866951\PG=C01 [X(C20H32Li1O8)]\\@

Chain Li+(Mon)$_3$

1\1\GINC-V1418\Freq\RM062X\6-31+G(d,p)\C21H36Li1O8(1+)\BXN501\30-Dec-2012\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) SCF=tight Freq=(noraman) maxdisk=1342177280\\MMA_chain_Li+.MMA3.freq\\1,1\Li,0.069902792,-0.0090405312,0.0605881882\O,0.0490963834,0.0280578909,1.969488084\O,1.9657495657,0.0992086594,-0.2837385089\O,-0.6564913019,-1.7034708687,-0.3341258398\O,-0.5915716008,1.437000066,-0.9513955266\C,-0.3415017639,2.5895830736,-1.2839015676\C,-0.4892466366,-2.9044703513,-0.496127996\C,3.006851262,0.0070772757,0.3585207523\C,-0.7115926331,-0.0472106314,2.9296742271\C,-2.1870007581,0.1085156558,2.8197362606\O,-0.2615151486,-0.2711978585,4.1539882091\C,1.1566000653,-0.4238956578,4.3003745779\H,1.3271074642,-0.5350252454,5.3685464816\H,1.494816923,-1.3113892664,3.7606052723\H,1.6729599139,0.4557921014,3.9115209896\C,-2.7112258144,0.4039662105,1.4430524395\H,-3.7979365977,0.4981673968,1.4652740796\H,-2.2894556786,1.3344279509,1.05010295\H,-2.4414871407,-0.3906739114,0.7390452237\C,-2.9505105223,-0.0188964536,3.9098477885\H,-4.0284772383,0.0905193307,3.8433611293\H,-2.5218692859,-0.2326137195,4.8822854692\O,-0.6225967734,3.0466896078,-2.4918875894\C,0.2847821483,3.5852084237,-0.3691466905\C,0.4729392884,3.1357273834,1.0523022385\H,0.9550375836,3.9209643201,1.6372468392\H,-0.4892382705,2.897443239,1.5177952944\H,1.0802166992,2.2259459842,1.1086300609\C,0.6353121742,4.7890099883,-0.8332176399\H,1.0929863097,5.5224812946,-0.1763453518\H,0.4692908211,5.0684239836,-1.8674399143\C,-1.2235929406,2.1192239894,-3.4074471967\H,-1.3849340743,2.681786567,-4.3236491276\H,-0.5491950509,1.2788143099,-3.5808923947\H,-2.1687337045,1.7552578972,-3.0019949189\O,0.203495178,-3.3832941704,-1.5177987267\C,-1.0809984171,-3.9793755926,0.3985206802\C,0.7260712974,-2.4227404544,-2.4482922479\H,1.2664488166,-3.0037298979,-3.1919243026\H,-0.095594062,-1.8711288502,-2.9096116122\H,1.3915606673,-1.7251652915,-1.9339300846\C,-0.0599339186,-5.1004034815,0.6365983524\H,-0.5100768408,-5.8610360472,1.2806670271\H,0.2406584225,-5.5729540455,-0.3003841926\H,0.836695693,-4.7217662619,1.1377512852\C,-1.5076974607,-3.3484675042,1.7259290625\H,-2.249318625,-2.5598819958,1.5741754267\H,-0.6495203486,-2.9168900388,2.2543442463\O,3.9719450027,0.9058729628,0.2636388421\C,3.7552271031,1.9996940599,-0.640418764\H,4.6690664891,2.5878303629,-0.6047319519\H,3.5771857321,1.6192692975,-1.6475569518\H,2.8994072808,2.594995354,-0.3165748945\C,3.301479047,-1.1241802869,1.2818151267\C,2.3607651185,-2.2924597965,1.1989536299\H,2.6573401533,-3.067992682,1.908650808\H,1.3359709904,-1.9767495044,1.4199315155\H,2.3644045986,-2.7290005673,0.1931621903\C,4.3488123081,-1.0537264716,2.1093205379\H,5.0033939393,-0.189613782,2.1233714709\H,4.572439319,-1.8705643178,2.789086053\H,-1.9480080737,-4.1165533945,2.3675683035\C,-2.3116961561,-4.5403223233,-0.3422075903\H,-2.7832616128,-5.3064149011,0.28002831\H,-3.0501551418,-3.7559365346,-0.5349075033\H,-2.0245001433,-4.9979759314,-1.2923995587\\Version=EM64L-G09RevA.02\State=1-A\HF=-1430.6152246\RMSD=5.480e-09\RMSF=4.717e-06\ZeroPoint=0.5582186\Thermal=0.5978595\Dipole=0.4631686,0.5666544,-0.1960222\\PG=C01 [X(C21H36Li1O8)]\\@

Rad-H Li+(Mon)$_3$

1\1\GINC-V1364\FOpt\RM062X\6-31+G(d,p)\C20H34Li1O8(1+)\BXN501\11-Sep-2013\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=671088640\\MMA_rad_H_Li+.MMA3.freq\\1,1\Li,-0.0519868048,0.021546707,-0.0222585167\O,-0.0289679438,0.0171345162,1.8853709628\O,1.8528909898,-0.0324084773,-0.3764414225\O,-0.8872190132,-1.6052921939,-0.4892495308\O,-0.5832647098,1.5621220063,-0.9662588972\C,-0.2457933559,2.7022459383,-1.2627926849\C,-0.7573502005,-2.812424968,-0.6347600427\C,2.8871117214,-0.2180801835,0.256171232\C,-0.7703109224,0.0049317517,2.8638147021\C,-2.2357015077,0.2452909904,2.7821012222\O,-0.3061687598,-0.2277161974,4.0809477921\C,1.1025300977,-0.4698302507,4.1970268913\H,1.2899465047,-0.5831916219,5.2621014198\H,1.3712825572,-1.380924344,3.6575114962\H,1.6645614416,0.3724593149,3.7889324005\C,-2.7682185541,0.5595214543,1.4129222345\H,-3.847006576,0.7168175342,1.4540815108\H,-2.3008296171,1.4610295988,1.0039103817\H,-2.5583525302,-0.2561266133,0.7127075989\C,-2.9832406515,0.1680218172,3.887940608\H,-4.0545048748,0.337203974,3.8418658107\H,-2.5476806772,-0.0632117838,4.8532893743\O,-0.497953243,3.2204316177,-2.4521479491\C,0.4626414606,3.6139352053,-0.3210158652\C,0.6245574986,3.101491591,1.0821682139\H,1.1696860953,3.8260056191,1.6896591333\H,-0.3505909758,2.9216287094,1.547204585\H,1.1596806661,2.1459195142,1.1006079203\C,0.9034615058,4.8018894552,-0.7473008868\H,1.4218462616,5.4742667495,-0.0704827467\H,0.7528420198,5.1287031799,-1.7699278292\C,-1.1763147654,2.3745107483,-3.3925114684\H,-1.2987702853,2.9788414661,-4.2878901928\H,-0.5715038295,1.490028248,-3.5999639093\H,-2.1445055522,2.0725215933,-2.9906669698\O,-0.1030799511,-3.3349301088,-1.6600438925\C,-1.324040809,-3.8574294935,0.2962672066\C,0.4431230011,-2.4114974267,-2.6150483673\H,0.9572094961,-3.0257188482,-3.3504736705\H,-0.363416615,-1.8429799041,-3.0820020789\H,1.1361204265,-1.7274922323,-2.1189515002\H,-0.5076689809,-4.5641150356,0.4916537078\C,-1.8012725237,-3.2290061709,1.6016416919\H,-2.6180032475,-2.5245364384,1.41786262\H,-0.9952512495,-2.6890550001,2.1087684268\O,3.916627649,0.6084353929,0.1768989383\C,3.7787474213,1.7356069794,-0.7009990026\H,4.7333888243,2.2541768718,-0.6557587487\H,3.5708677036,1.3926565474,-1.715860343\H,2.9699023138,2.38

48256023,-0.3602775495\C,3.1014658093,-1.3915376744,1.1490409472\C,2.0617078274,-2.47215899,1.060286582\H,2.3021504138,-3.2899840067,1.7427531998\H,1.075134254,-2.0714801377,1.3137410564\H,2.0069115898,-2.8776978204,0.0434855475\C,4.1675086836,-1.4311846468,1.9543837973\H,4.8942871217,-0.6269297658,1.9733122578\H,4.3339769957,-2.2808013441,2.6099276189\H,-2.1667384788,-4.0072838366,2.2755473589\C,-2.4529404115,-4.6153747726,-0.4235838289\H,-2.8446258451,-5.395055097,0.2336134728\H,-3.2748847194,-3.9358371699,-0.6696489896\H,-2.0957571885,-5.0842220556,-1.3423509754\\Version=ES64L-G09RevD.01\State=1-A\HF=-1391.3163361\RMSD=4.392e-09\RMSF=1.029e-05\Dipole=0.4445653,0.2980143,-0.1503402\Quadrupole=-3.752715,2.0684405,1.6842745,5.1239736,1.2817572,-6.8893856\PG=C01 [X(C20H34Li1O8)]\\@

Polymer Binding Selectivity

Di-rad

1\1\GINC-V1377\Freq\UM062X\6-31+G(d,p)\C10H17O4(2)\BXN501\01-Mar-2013\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) SCF=tight Freq=(noraman) maxdisk=268435456\\MMA_dimer_rad.2.freq\\0,2\C,0.0073426081,0.0153732414,0.021776638\H,-0.0213562238,0.0031034363,1.1149001322\H,1.0471294479,0.0570553549,-0.3129708616\H,-0.4187079993,-0.9221079349,-0.3452833376\C,-0.7719419475,1.2228898484,-0.4973113943\C,-0.085864907,2.529935268,-0.070449784\H,-0.6512717377,3.402529325,-0.4067124936\H,-0.0093701011,2.5586826784,1.0207920555\H,0.9261279239,2.5896197002,-0.4834535378\C,-0.8164741514,1.1715338637,-2.0197651959\C,-2.2267965546,1.2244426924,0.0614013078\H,-2.7405292032,2.1099253177,-0.331376027\H,-2.1518020197,1.3121476096,1.1494530339\C,-3.0102812805,0.0008908247,-0.2801616766\O,-0.3084514558,0.3200590128,-2.7110042025\O,-1.5073500581,2.2055197656,-2.5386875458\C,-1.6165491629,2.2128815837,-3.9629958765\H,-2.1856181007,3.1068208406,-4.2118890812\H,-0.6255869036,2.2438103197,-4.4201159617\H,-2.1372048695,1.3149015515,-4.3055863412\C,-3.5793432802,-0.1913257985,-1.6464782501\H,-4.4823001827,-0.8041046258,-1.6201166515\H,-3.8025578176,0.7755809924,-2.1073262117\H,-2.8594750197,-0.7090545715,-2.298584598\C,-3.1231455386,-1.0348393682,0.7368383001\O,-2.6545524137,-0.9576605917,1.8616917251\O,-3.810740507,-2.1204316733,0.3125399073\C,-3.9443685759,-3.1630394652,1.2765199069\H,-4.5127833402,-3.9497320318,0.7832361751\H,-2.9610182375,-3.5292788367,1.5796987521\H,-4.4737803542,-2.7995335024,2.1601361463\\Version=EM64L-G09RevA.02\State=2-A\HF=-691.9182238\S2=0.758255\S2-1=0.\S2A=0.750048\RMSD=7.770e-09\RMSF=6.465e-07\ZeroPoint=0.2641095\Thermal=0.2808691\Dipole=-0.5813047,0.4736175,-0.5708119\PG=C01 [X(C10H17O4)]\\@

Di-rad[a]

1\1\GINC-V1388\Freq\UM062X\6-31+G(d,p)\C10H17O4(2)\BXN501\01-Mar-2013\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) SCF=tight Freq=(noraman) maxdisk=268435456\\MMA_dimer_rad.3.freq\\0,2\C,0.0081899972,0.0184899952,0.0071859054\H,-0.0622813203,-0.0254975941,1.0985966702\H,1.0631794372,0.0996639512,-0.2693135133\H,-0.3758074496,-0.9129748382,-0.4140522798\C,-0.7796009312,1.2220648323,-0.5122981124\C,-0.2277966602,2.5201666963,0.0877278092\H,-0.7568175096,3.3990911671,-0.2851550154\H,-0.3193792041,2.4882735903,1.1790016993\H,0.8326294505,2.6343970244,-0.1580693679\C,-0.686754101,1.2426853893,-2.0357285485\C,-2.2837689635,1.021281548,-0.1318896286\H,-2.311357611,0.8931295023,0.9577482662\H,-2.6223413708,0.0899605363,-0.5983653235\C,-3.2028161061,2.1312635552,-0.5179163187\O,-0.3596542185,0.3032390698,-2.7194609478\O,-1.0360167186,2.4356203242,-2.5510128106\C,-1.135254205,2.4681698449,-3.9775170681\H,-1.4366759599,3.4847719889,-4.2273512465\H,-0.1706897798,2.2294740553,-4.4298700183\H,-1.8846185988,1.743930931,-4.30570561\C,-3.453201081,3.3086502483,0.3639058166\H,-4.5228755569,3.4162066824,0.5792681819\H,-2.9105896558,3.2167358421,1.3069102899\H,-3.147309877,4.2405361327,-0.1276757411\C,-3.8471444413,2.0455414498,-1.8188411557\O,-3.6987950685,1.1278596366,-2.610284598\O,-4.6437574671,3.1080518162,-2.080068358\C,-5.2965045153,3.0732584804,-3.3475015648\H,-5.8930332867,3.9825933084,-3.3983324502\H,-4.5602722192,3.050266648,-4.1546534784\H,-5.9322561225,2.1885738328,-3.4254879757\\Version=EM64L-G09RevA.02\State=2-A\HF=-691.9178173\S2=0.757788\S2-1=0.\S2A=0.750044\RMSD=6.931e-09\RMSF=4.649e-06\ZeroPoint=0.2643386\Thermal=0.28085\Dipole=-0.4129256,1.211117,0.6268913\PG=C01 [X(C10H17O4)]\\@

Di-chain

1\1\GINC-V1382\Freq\RM062X\6-31+G(d,p)\C11H20O4\BXN501\16-May-2013\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) SCF=tight Freq=(noraman) maxdisk=268435456\\MMA_dimer_chain.2.freq\\0,1\H,-0.9687675398,-2.0103654817,2.8927075556\C,-0.709489909,-0.9685776929,2.6786846348\H,-0.9815674711,-0.7552266281,1.6402699947\H,0.3716107062,-0.8469792154,2.7888960227\C,-1.475971891,-0.0100608939,3.6139420056\C,-0.9891701894,1.4245032944,3.313179796\C,-2.9801453226,-0.1849254652,3.3934973062\H,-3.2386164394,0.1312784631,2.3777259992\H,-3.2631300538,-1.2326337771,3.520335169\H,-3.5718235754,0.3958912646,4.1069009983\C,-1.134037148,-0.4483787379,5.0342635812\O,0.1407337726,-0.1628903316,5.3621108987\C,0.5369337303,-0.5679320286,6.6734300659\H,-0.0825420417,-0.0703189015,7.423790021\H,0.430312957,-1.6488876833,6.7861254374\H,1.5790436875,-0.2690708981,6.773562511\O,-1.8806780487,-1.0339387181,5.7827578997\C,-1.6952856768,2.6120960493,4.0035266778\H,-1.0612393145,1.5706225301,2.229301654\H,0.0738071917,1.4836075325,3.573815896\C,-1.7575466092,2.4625300333,5.5251996884\C,-0.9095599884,3.8919405838,3.6494040225\H,0.0949494716,3.8304229401,4.0795568313\H,-0.8192571562,4.0126959449,2.5663570405\H,-1.4037676975,4.7778198125,4.0609183602\C,-3.1090998913,2.8286038244,3.4736840257\O,-4.0814820315,3.0585846752,4.1535264875\O,-3.1590410576,2.796539819,2.1282013475\C,-4.4520291411,3.0162308923,1.5620080379\H,-4.316080605,2.9618949186,0.4831684867\H,-4.8348005828,3.9956591601,1.8564877149\H,-5.1478935198,2.2460240301,1.9040138044\H,-2.1734146335,3.3654434695,5.9786910921\H,-0.7479694297,2.3020458042,5.917106247\H,-2.3936585523,1.6272434113,5.8317076888\\Version=EM64L-G09RevA.02\State=1-A\HF=-731.8627919\RMSD=5.963e-09\RMSF=8.561e-05\ZeroPoint=0.3061685\Thermal=0.3237889\Dipole=0.9677671,0.2003195,-0.8042929\PG=C01 [X(C11H20O4)]\\@

Di-rad Li+

1\1\GINC-V1280\Freq\UM062X\6-31+G(d,p)\C10H17Li1O4(1+,2)\BXN501\29-Dec-2012\0\\#M062X/6-31+G(d,p) I
NT(grid=ultrafine) SCF=tight Freq=(noraman) maxdisk=268435456\\MMA_dimer_rad_Li+.A.freq\\1,2\C,-0.0402361
869,-0.0400953417,-0.029923589\H,-0.0483304572,-0.0504905526,1.063697341\H,0.9993668634,-0.0350761074,-0.
3604256608\H,-0.5046824216,-0.9615698044,-0.3917083807\C,-0.7715768828,1.2102841084,-0.5304969322\C,0.00
88223989,2.4725414725,-0.0980188504\H,-0.4956590269,3.3883235682,-0.4197511784\H,0.0897358732,2.4873980
011,0.9923054995\H,1.0200135657,2.4624891756,-0.5128842422\C,-0.7923172694,1.2619445937,-2.0507663057\C,
-2.2123624874,1.3184080152,0.0432813533\H,-2.68181773,2.2287238919,-0.3423412153\H,-2.0900463295,1.46531
13801,1.124091227\C,-3.1217992532,0.1440870725,-0.1498566319\O,-1.6413300025,1.8577897036,-2.7156199477\
O,0.2379531465,0.6840130638,-2.6145093256\C,0.365946082,0.7877454575,-4.0476102842\H,1.2858756909,0.262
5542408,-4.2895292786\H,-0.4906257495,0.3141132011,-4.5282026814\H,0.4266812115,1.8377506034,-4.3353540
608\C,-3.0425654817,-1.0555352181,0.7339025918\H,-2.9003216021,-1.9735375629,0.1517368602\H,-2.232270619
,-0.9661910296,1.4566334847\H,-3.9857776738,-1.1885184952,1.2771567014\C,-4.2175147866,0.2277207736,-1.10
18385413\O,-4.4171224684,1.176669576,-1.8810590313\O,-5.0291390727,-0.8136245301,-1.065813256\C,-6.15594
57586,-0.8035286705,-1.95990403\H,-6.6953329899,-1.7233020297,-1.7495982353\H,-6.7789858669,0.0691588635,
-1.7605346836\H,-5.8086669918,-0.7854129735,-2.9940241567\Li,-3.3764144659,2.3300587036,-2.7638996031\\Ve
rsion=EM64L-G09RevA.02\State=2-A\HF=-699.3210022\S2=0.755626\S2-1=0.\S2A=0.750026\RMSD=7.348e-09\R
MSF=4.781e-06\ZeroPoint=0.2680112\Thermal=0.2854668\Dipole=-0.5367527,0.8243841,-1.033457\PG=C01 [X(C1
0H17Li1O4)]\\@

Di-chain Li+

1\1\GINC-V1255\Freq\RM062X\6-31+G(d,p)\C11H20Li1O4(1+)\BXN501\22-Dec-2012\0\\#M062X/6-31+G(d,p) IN
T(grid=ultrafine) SCF=tight Freq=(noraman) maxdisk=268435456\\MMA_dimer_chain_Li+.1.freq\\1,1\H,-0.1787615
503,-0.3200908667,0.0964102977\C,-0.2563420322,-0.3097322191,1.1872486753\H,0.7099563651,-0.6157100288,1.
5971461311\H,-1.0096272228,-1.0392162846,1.4876238587\C,-0.5952590588,1.103171114,1.7007471439\C,-0.7049
538457,1.0072201046,3.252653543\C,0.5161532613,2.0587412454,1.2445162682\H,1.4628934523,1.7454250914,1.
6928754713\H,0.6288803903,2.0205888024,0.1576763192\H,0.3435525713,3.100745011,1.5183310246\C,-1.928629
2523,1.5432724404,1.1182913896\O,-2.8303133638,0.59361712,1.0842757964\C,-4.1404716683,0.926365326,0.583
7794613\H,-4.6101175828,1.6594263825,1.2426700397\H,-4.0585260314,1.3272973902,-0.426518141\H,-4.694834
5143,-0.0082047226,0.5909743506\O,-2.1813760677,2.6872535749,0.7307781388\C,-1.2848699252,2.1602280546,4
.1265627146\H,0.3121044965,0.796222674,3.6030389063\H,-1.3108976106,0.1263675803,3.4948012038\C,-2.8078
306121,2.2965364332,3.9905918953\C,-0.9613066877,1.8168859753,5.5936314811\H,-1.4585956181,0.8799029654
,5.8584549576\H,0.1114060448,1.699842715,5.7529945702\H,-1.329206107,2.596260009,6.266892025\C,-0.611978
4615,3.4723820533,3.7573398035\O,-1.1200987732,4.3464126836,3.0498270475\O,0.6002074123,3.5987847963,4.
2376276849\C,1.3340326386,4.7947815222,3.9079104528\H,2.27127265,4.7139742212,4.4518320039\H,0.7702458
325,5.6724796365,4.2240730334\H,1.5137118171,4.8304985763,2.8315551344\H,-3.1873224847,3.0452828807,4.6
911382478\H,-3.2752189547,1.3387564083,4.2349609071\H,-3.1388426639,2.586439614,2.9921100886\Li,-1.95979
11167,4.3389078134,1.4436165238\\Version=EM64L-G09RevA.02\State=1-A\HF=-739.2606163\RMSD=8.277e-09\
RMSF=9.233e-06\ZeroPoint=0.3095289\Thermal=0.3281913\Dipole=-0.4903309,1.3031567,-0.7082741\PG=C01 [X(
C11H20Li1O4)]\\@

Di-rad Li+(Mon)

1\1\GINC-V1428\Freq\UM062X\6-31+G(d,p)\C15H25Li1O6(1+,2)\BXN501\06-Jan-2013\0\\#M062X/6-31+G(d,p) I
NT(grid=ultrafine) SCF=tight Freq=(noraman) maxdisk=2013265920\\MMA_dimer_rad_Li+.A.MMA.freq\\1,2\C,0.2
709714169,0.4641026379,0.699227616\C,0.2620327968,-0.1340741447,2.1097551232\C,1.6904635055,-0.48456238
8,2.6108476981\C,2.5019331081,-1.3981152395,1.7472598114\C,2.7144995484,-2.7747829554,2.1660285033\O,3.5
386354954,-3.4433778674,1.3691040301\C,3.8176617963,-4.8070571984,1.7211497519\C,-0.3550926363,0.880132
3938,3.0968414247\C,-0.6319520084,-1.3638611573,2.1836716205\O,-1.6217545447,-1.3499431423,1.3173563073\
C,-2.5776645155,-2.4241269134,1.3918703601\O,-0.5105158609,-2.2590209463,3.0125982553\C,3.2285573,-0.8984
215535,0.54311113\O,2.2121149858,-3.3027397383,3.1671846684\Li,0.600836922,-3.3134964686,4.050573418\O,0
.1852285786,-4.1880285511,5.6204704835\C,0.3001441504,-4.0147749409,6.8335578415\O,-0.08231084,-4.920282
6711,7.7068900489\C,-0.6427632189,-6.1367699429,7.183319549\C,0.8761843424,-2.7721448816,7.4113310485\C,
1.3092843151,-1.7427611034,6.4047097181\C,0.9799951137,-2.6306774746,8.7355266878\H,0.9403770624,1.3290
629518,0.6760363285\H,-0.7282036081,0.8000975861,0.4178121115\H,0.6062728563,-0.2570251541,-0.051054839
1\H,-0.3577391421,0.4918931506,4.1197522419\H,0.2310707911,1.803259837,3.0783761893\H,1.6154832719,-0.89
75601801,3.6209441805\H,2.225871272,0.4706070905,2.688504923\H,-3.3089999253,-2.2108870183,0.6167159243
\H,-2.0788505579,-3.3758426262,1.2047370524\H,-3.0435929043,-2.4358081706,2.377907667\H,2.9251333311,-1.4
396339574,-0.3609281553\H,3.0588615138,0.1670560103,0.3890734855\H,4.3057412301,-1.072763176,0.64893137

27\H,4.5157120051,-5.161464593,0.9668824326\H,4.2628085292,-4.8513261156,2.7161339846\H,2.8971449232,-5.3928712445,1.7029257582\H,1.7045377662,-0.8575059473,6.9048313964\H,2.0936167965,-2.1401975396,5.74872583\H,0.4622075043,-1.4292213569,5.7811245051\H,1.3990501754,-1.7265963895,9.1658142519\H,0.6515353093,-3.4099672429,9.4139114199\H,-0.8895361831,-6.736614266,8.0554439108\H,-1.5359869666,-5.9110789815,6.5994379536\H,0.0929399024,-6.6430942855,6.5571390878\H,-1.38161606,1.1238130639,2.8102911057\\Version=EM64L-G09RevA.02\State=2-A\HF=-1045.016392\S2=0.756001\S2-1=0.\S2A=0.750029\RMSD=6.791e-09\RMSF=4.453e-06\ZeroPoint=0.3941979\Thermal=0.4214534\Dipole=-0.1914597,-0.3383336,0.0691582\PG=C01 [X(C15H25Li1O6)]\\@

Di-chain Li+(Mon)

1\1\GINC-V1474\Freq\RM062X\6-31+G(d,p)\C16H28Li1O6(1+)\BXN501\24-Dec-2012\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) SCF=tight Freq=(noraman) maxdisk=671088640\\MMA_dimer_chain_Li+.1.MMA.freq\\1,1\H,-0.1214587322,0.4635192069,-0.411251189\C,0.0259218491,0.3926207348,0.6702495786\H,1.093625381,0.5128290528,0.8740588172\H,-0.2819875277,-0.6017546676,0.996636591\C,-0.7546661295,1.49879378,1.4049724588\C,-0.5032196158,1.2980653066,2.9289990679\C,-0.2596169122,2.859944466,0.8971606387\H,0.7940478392,2.9824522153,1.1633082884\H,-0.3419903695,2.9086501746,-0.1927124215\H,-0.8191824244,3.7048715903,1.3011485107\C,-2.2391437346,1.3521482418,1.1124921401\O,-2.6567319643,0.1038778862,1.1401023666\C,-4.0592639632,-0.1296401836,0.9208144201\H,-4.6405826282,0.3296424643,1.7232014916\H,-4.3590440292,0.2883569732,-0.0404881406\H,-4.1761117838,-1.2101992869,0.9316550841\O,-3.0069748993,2.2867782319,0.8984474936\C,-1.3321725406,2.0512000703,4.0113188797\H,0.5552298376,1.5367838953,3.085943578\H,-0.6241495338,0.232094896,3.1547242262\C,-2.7621165939,1.5103166586,4.1456654811\C,-0.6099492931,1.8461957395,5.3564768957\H,-0.5961197552,0.7791132967,5.595294792\H,0.4180909297,2.2093712389,5.3207954699\H,-1.1338337527,2.3660110611,6.1637050745\C,-1.3713050111,3.5337055026,3.6779476144\O,-2.3326810361,4.1188119386,3.1870485511\O,-0.2392719132,4.1564317276,3.9350107961\C,-0.1629165632,5.5528712923,3.6020956097\H,0.8081908589,5.882878122,3.9620556109\H,-0.9700276087,6.0975999883,4.0927353657\H,-0.2336171112,5.676875891,2.5188001938\H,-3.2697568158,1.9875925372,4.9883295005\H,-2.7228940003,0.434599456,4.3381656729\H,-3.3785010097,1.6745902942,3.2607912459\Li,-3.5351900337,3.8486136911,1.7868967073\O,-4.877787597,4.9664727822,1.2107855483\C,-5.0010847093,5.8871683507,0.4026314357\O,-6.1502306637,6.4952571166,0.209178483\C,-7.2703236719,6.0394784254,0.9879911468\H,-8.1044097479,6.6659811123,0.6829243331\H,-7.4702711834,4.9898916459,0.7687093895\H,-7.0567627507,6.163789858,2.0503372222\C,-3.8659298838,6.3871314919,-0.4169292258\C,-4.0531956234,7.3821515806,-1.2883570396\C,-2.5532601806,5.6929288168,-0.1798100444\H,-3.2308021517,7.7533177645,-1.8917100515\H,-5.0255775623,7.843703329,-1.4179569265\H,-1.7707978185,6.1255735494,-0.805013 1116\H,-2.2429395568,5.7943871866,0.8683482963\H,-2.6217563514,4.6240399696,-0.415749351\\Version=EM64L-G09RevA.02\State=1-A\HF=-1084.9573003\RMSD=3.119e-09\RMSF=3.776e-06\ZeroPoint=0.4359825\Thermal=0.46424\Dipole=-0.4237684,0.3296095,-0.1864456\PG=C01 [X(C16H28Li1O6)]\\@

Di-rad Li+(Mon)$_2$

1\1\GINC-V1358\Freq\UM062X\6-31+G(d,p)\C20H33Li1O8(1+,2)\BXN501\26-Dec-2012\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) SCF=tight Freq=(noraman) maxdisk=1342177280\\MMA_dimer_rad_Li+.A.MMA2.freq\\1,2\C,0.0571857354,-0.0266637105,-0.0198267273\C,0.0652864116,-0.0039373467,1.5122400585\C,1.5020914487,-0.0394651602,2.0993275745\C,2.3453536752,-1.2167695828,1.7274291899\C,2.6190426666,-2.2289488603,2.7359619725\O,3.4231843782,-3.1988414062,2.3039895998\C,3.7510341241,-4.2232645271,3.2519126067\C,-0.6180045295,1.2853768229,2.013016108\C,-0.748939904,-1.1554634756,2.0885419198\O,-1.7403908752,-1.5399220104,1.3026975067\C,-2.6112471457,-2.5617807531,1.8156748731\O,-0.56980486,-1.6484848174,3.191074717\C,3.0234943339,-1.3191976707,0.4016322201\O,2.1885318361,-2.2142157004,3.8930666738\Li,0.5376648216,-1.8225340669,4.748893958\O,0.0756786891,-3.2715485971,5.8553213166\C,0.4482476707,-3.9696800552,6.7911693125\O,-0.1948139789,-5.0737188085,7.1356267367\C,-1.3519100302,-5.4125283219,6.3598559555\C,1.6401442635,-3.652067962,7.6245648981\C,2.3415622472,-2.3685352479,7.2819786585\C,2.012932092,-4.485204635,8.6007144994\O,0.3831084694,-0.1347203411,5.5989092438\C,0.5078945926,1.0835178263,5.5697698299\C,1.8190249952,1.7568997861,5.3612628053\C,3.0282445181,0.8768524814,5.510130047\O,-0.5264262523,1.8975150708,5.7105067298\C,-1.8087851926,1.2757542451,5.885543381\C,1.8528797213,3.0555881383,5.0457530119\H,0.6886349715,0.7825069083,-0.3991797118\H,-0.9544284107,0.122166562,-0.4010583235\H,0.4278051847,-0.97446457,-0.4188000118\H,-0.6108592228,1.3412597694,3.1064692766\H,-0.0806477838,2.1554133338,1.6240436048\H,1.4282440685,0.0275895342,3.1879210485\H,2.0020202329,0.8726008221,1.7460577036\H,-3.3460588838,-2.7342570409,1.0332538694\H,-2.0392005645,-3.4676850462,2.0209879173\H,-3.0904853075,-2.2151376461,2.7325796573\H,2.6790004007,-2.1986389976,-0.1564049565\H,2.8474985283,-0.4302961952,-0.2045491284\H,4.1032097337,-1.4521123899,0.5326084386\H,4.391269936,-4.9198283715,2.7159115079\H,4.2784188737,-3.7896202237,4.1037543308\H,2.8417570717,-4.7180233906,3.5986431529\H,3.1830982955,-2.2049448232,7.9574311957\H,2.7144606578,-2.3880614754,6.2521033429\H,1.6555499152,-1.5187340251,7.360828948\H,2.8792956261,-4.2621681269,9.2155627861\H,1.4664636438,-5.39828915

98,8.8072388555\H,-1.7315429471,-6.3339309107,6.7947545444\H,-2.0937411005,-4.6153441585,6.4295233539\H,-1.0709801933,-5.5623497923,5.3159414714\H,-2.5210659328,2.0949619561,5.9456244968\H,-2.0290535795,0.6254841369,5.0355905246\H,-1.8135697126,0.6877366191,6.8044899956\H,3.9326381139,1.4248768692,5.2416813579\H,3.1266477822,0.532416104,6.545012614\H,2.9495245246,-0.0189894417,4.8854096529\H,2.7993466877,3.5568817541,4.8681347323\H,0.9446965214,3.6425166878,4.9637653334\H,-1.6527017565,1.3381616333,1.6629731675\\Version=EM64L-G09RevA.02\State=2-A\HF=-1390.697892\S2=0.756343\S2-1=0.\S2A=0.750032\RMSD=4.282e-09\RMSF=6.644e-06\ZeroPoint=0.5202965\Thermal=0.5572098\Dipole=-0.3521855,-0.1759473,-0.3469392\PG=C01 [X(C20H33Li1O8)]\\@

Di-chain Li+(Mon)$_2$

1\1\GINC-V1409\Freq\RM062X\6-31+G(d,p)\C21H36Li1O8(1+)\BXN501\07-Jan-2013\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) SCF=tight Freq=(noraman) maxdisk=1610612736\\MMA_dimer_chain_Li+.1.MMA2.freq\\1,1\H,1.5389550312,-3.0565438328,-3.2142627807\C,1.8911718331,-3.3170231119,-2.211954881\H,2.9780288153,-3.4327388844,-2.2552802707\H,1.4491443156,-4.273335248,-1.92774696\C,1.5415412316,-2.2087330966,-1.2016648945\C,2.047910759,-2.6819154945,0.1912395455\C,2.2004293655,-0.9001002057,-1.6596703665\H,3.2880629494,-0.99617294,-1.5905637722\H,1.9386121762,-0.6972899502,-2.7025870813\H,1.8806957027,-0.0328127006,-1.0789238024\C,0.0345567009,-2.0189403195,-1.1589108829\O,-0.638154919,-3.1577684054,-1.1180590421\C,-2.0661067866,-3.0576228074,-1.0069157786\H,-2.3313462962,-2.612309103,-0.0431665257\H,-2.4656785384,-2.4429750938,-1.8152396486\H,-2.4360430476,-4.0781116274,-1.0698263211\O,-0.5318193496,-0.9353788748,-1.1349007775\C,1.6364266814,-1.9507473984,1.5012783048\H,3.1423904921,-2.6751072072,0.1270702765\H,1.7445635257,-3.726751649,0.3265776481\C,0.1721325631,-2.2027479269,1.8869609234\C,2.5419715849,-2.4887622914,2.6245854234\H,2.3601374058,-3.5601501098,2.7494364718\H,3.5981755343,-2.3380790942,2.3956294148\H,2.3194765028,-1.995323922,3.575134494\C,1.8593545496,-0.4560801235,1.3428245402\O,0.9705320076,0.369488005,1.1882518092\O,3.1366521354,-0.1103866446,1.3559955039\C,3.4291111068,1.2789514331,1.1424153561\H,4.5051527816,1.3731673004,1.2667512058\H,2.8932788378,1.8935196814,1.8677003297\H,3.1334082438,1.5672994148,0.1290712842\H,-0.0216880264,-1.8074421143,2.8887227319\H,-0.0213818137,-3.279483605,1.8987535376\H,-0.5380370414,-1.7193994963,1.2133965559\Li,-0.5003818409,0.6605533454,-0.0378412272\O,0.214147902,2.1450247583,-0.9628386722\O,-2.1794019899,0.4417935679,0.7996662458\C,0.8452881976,3.1368290351,-0.612505618\C,-3.2779074541,0.0629559311,0.406546822\O,-4.0843294116,-0.647959079,1.1797067274\C,-3.614578999,-0.937980246,2.5043316295\H,-4.4172499322,-1.4963130041,2.9798713925\H,-2.7014583916,-1.535436499,2.4548931206\H,-3.4135370088,-0.0097543631,3.0410065702\C,-3.8120207568,0.3631511534,-0.9502109175\C,-4.9976575059,-0.1318078276,-1.3207103115\C,-2.9477336395,1.2378737555,-1.8138948977\H,-5.4033731649,0.0866718266,-2.3036450729\H,-5.5869259142,-0.7538688919,-0.6564311242\H,-3.4746597393,1.4971055473,-2.7333870513\H,-2.6806583608,2.1631929415,-1.2939681618\H,-2.0161638831,0.7297363663,-2.082303688\O,1.7946767248,3.659688836,-1.3732990814\C,0.6097374734,3.8467396955,0.6746122204\C,1.3773489424,4.8900003625,1.0068065657\C,-0.5185839292,3.3187910725,1.515001524\H,1.2107486013,5.4225581102,1.9380036074\H,2.1762545355,5.2367236763,0.3610535245\H,-0.6877202149,3.9727980893,2.3717300739\H,-1.4453887112,3.258185642,0.9360082335\H,-0.2960810127,2.3138724378,1.8874208072\C,2.0355640077,3.0170446993,-2.6336005903\H,2.8183339968,3.6013822525,-3.1110707984\H,2.3625264545,1.9874051638,-2.4719936199\H,1.1249957359,3.0196757829,-3.2343599759\\Version=EM64L-G09RevA.02\State=1-A\HF=-1430.641145\RMSD=4.908e-09\RMSF=6.365e-06\ZeroPoint=0.5624371\Thermal=0.6000616\Dipole=0.0141996,-0.0197778,0.0011585\PG=C01 [X(C21H36Li1O8)]\\@

Di-rad Li+(Mon)$_3$

1\1\GINC-R171\Freq\UM062X\6-31+G(d,p)\C25H41Li1O10(1+,2)\ROOT\02-Nov-2013\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) SCF=tight Freq=(noraman) maxdisk=3489660928\\MMA_dimer_rad_Li+.radC.MMA3.9.freq\\1,2\Li,0.8102975314,0.2179186671,-0.1077757876\O,0.8134223475,-0.9769037272,1.3932845254\O,2.1901244361,-0.6580249966,-1.1478660773\O,-0.8813183417,0.2023331708,-0.9082144055\O,1.4680660563,1.9901190613,0.0364037826\C,2.5369892482,2.5886431555,0.065386903\C,-1.573236287,-0.4679751392,-1.6862944473\C,2.7378724148,-1.7542543888,-1.1968931\C,0.311524855,-1.1685541673,2.4968692135\C,-0.5480039254,-0.1671469153,3.1826275935\O,0.5044006729,-2.2959954781,3.1612326578\C,1.3185975675,-3.2876849975,2.5198501786\H,1.3882900453,-4.1083290749,3.2298137174\H,0.8469288387,-3.6158271969,1.5911440329\H,2.3063274804,-2.8778618354,2.2994391415\C,-0.6626359903,1.1600312266,2.4899168647\H,-1.3456455945,1.8165059735,3.0325869485\H,0.3133166267,1.6505754224,2.4132000085\H,-1.0484252193,1.0411496491,1.4716322615\C,-1.1646825912,-0.4893481636,4.3243945482\H,-1.8036307399,0.2300516857,4.8275251346\H,-1.0465595909,-1.4670667782,4.7776510478\O,2.7320870852,3.7076589629,-0.6122233814\C,3.7069695759,2.1347310369,0.8687683452\C,3.4617119646,0.9573920818,1.7696121211\H,4.376202697,0.6919832271,2.3033328198\H,2.6847071403,1.1850512479,2.5070743109\H,3.1131528893,0.0871511975,1.203592954\C,4.8767902876,2.7730040808,0.7620757312\H,5.7360578749,2.4525077027,1.3434973959\H,5.0000929362,3.6249506952,0.1031692758\C,1.6304082111,4.1846966309,-1.3970880462\H,1.9982679765,5.0744657958,-1.9020940633\H,1.32661979,3.4235869778,-2.1179464201\H,0.7902767246,4.4296098952,-0.7448864219\O,-1.3170122

223,-0.527277264,-2.9908163125\C,-2.7182377809,-1.2533969497,-1.2740733028\C,-0.265233718,0.3188242311,-3.4683586747\H,-0.2226237454,0.1512271259,-4.5422940376\H,-0.5101723822,1.3611365252,-3.2510854793\H,0.6824055791,0.0526133318,-2.9927594179\C,-3.1833709555,-1.0808597146,0.1320431677\H,-3.6757715447,-1.9963367224,0.4793747224\H,-2.322546422,-0.8832772268,0.7825831644\C,-4.2150748123,0.0870990437,0.3295076398\C,-3.453414099,-2.0701155125,-2.2793338656\H,-4.2485286555,-2.651083683,-1.8096302225\H,-2.7770446131,-2.7501234458,-2.8092492078\O,4.0480812177,-1.8776162268,-1.3342332962\C,4.8091875635,-0.6650766788,-1.432459017\H,5.8356106973,-0.9821900641,-1.6006057313\H,4.4464645631,-0.063825424,-2.2678180451\H,4.727920416,-0.0919979744,-0.507088081\C,2.0002429326,-3.0480347011,-1.1335830495\C,0.5052913217,-2.9565746345,-1.2513744227\H,0.0614032989,-3.9539332237,-1.2221012114\H,0.0869376064,-2.3569421051,-0.4362754484\H,0.218725383,-2.4803775023,-2.1957706879\C,2.6773807138,-4.1915627579,-0.988732741\H,3.7592070871,-4.2064131779,-0.9202618103\H,2.1532301408,-5.1414974369,-0.9414960323\H,-3.8972760689,-1.4207686618,-3.0453072513\C,-4.4559898348,0.2618301302,1.8299733444\C,-5.5288569365,-0.2242748952,-0.395095335\C,-3.5892443071,1.3214512913,-0.3146945793\H,-5.1340753096,1.0979549026,2.0210655186\H,-4.9129631348,-0.6470858629,2.2336148768\H,-3.5218331095,0.4494479395,2.3660578457\H,-6.2660207315,0.5589972977,-0.1961725351\H,-5.3881370079,-0.2807922119,-1.4757279435\H,-5.9375497577,-1.1732318257,-0.0339286179\O,-2.9839169875,2.1291604876,0.5620270167\O,-3.5803967795,1.5213381018,-1.5096901544\C,-2.2162644089,3.1921703964,-0.0125090972\H,-1.8188935512,3.7553076757,0.8311937201\H,-1.4058224441,2.7670015609,-0.6123089872\H,-2.8499201942,3.8237271568,-0.6373417841\\Version=ES64L-G09RevD.01\State=2-A\HF=-1736.3646285\S2=0.755602\S2-1=0.\S2A=0.750026\RMSD=5.676e-09\RMSF=3.906e-06\ZeroPoint=0.6463458\Thermal=0.6925829\Dipole=1.9032624,-0.5572399,0.4112038\PG=C01 [X(C25H41Li1O10)]\\@

Pro-meso/ Pro-racemo Selectivity

Tri-rad (pro-r)

1\1\GINC-R554\Freq\UM062X\6-31+G(d,p)\C15H25O6(2)\ROOT\04-Feb-2014\0\\#N Geom=AllCheck Guess=TChec
k SCRF=Check Test GenChk UM062X/6-31+G(d,p) Freq\\MMA_trimer_rad.a0b3d3.freq\\0,2\C,-1.2803965715,7.6264
213164,2.1832108876\H,-2.3150575233,7.9547500045,2.3162816158\H,-1.1505407389,7.2205234327,1.1760584678\
H,-0.6289740654,8.4995471282,2.2594544967\C,-0.9273758998,6.5924844818,3.2527337308\C,-1.8652828827,5.364
3014624,3.2376392677\H,-1.4920711939,4.6428316494,3.9735155534\H,-2.8471740338,5.7014405053,3.5873786444
\C,-2.0703907979,4.5992083532,1.911597029\C,0.5355222306,6.1923060969,3.09135107\C,-1.0672691567,7.228265
3362,4.678673889\H,-0.8744586518,6.4410176457,5.4179178932\H,-2.106102294,7.5580657683,4.774317933\C,-0.1
607954605,8.38424768,4.9408406286\O,1.3329324466,6.7374575595,2.3650126145\O,0.881181925,5.1777665314,3.
9086506401\C,2.2491937142,4.7737510941,3.828016065\H,2.3592001534,3.9560301858,4.5381075508\H,2.4844826
127,4.4420592222,2.8139446861\H,2.9068657396,5.6063811692,4.0896218734\C,1.2683780773,8.1903437834,5.326
1037833\H,1.9318144548,8.3849335956,4.472081623\H,1.5610871894,8.8860733854,6.1174154561\H,1.4411775302,
7.1643311721,5.6623371087\C,-0.7078146107,9.7235276567,4.7743138736\O,-1.8610761626,9.9710157645,4.459368
3801\O,0.2048805641,10.6939695661,5.0085672706\C,-0.2789100095,12.0268390382,4.8536372899\H,0.5674027638
,12.6752793649,5.0738204221\H,-0.6322503678,12.1868293605,3.8325573498\H,-1.1019267686,12.2164314758,5.54
63607848\C,-2.9178775693,3.3481575468,2.2242193523\C,-2.8772455686,5.4091520798,0.900709238\C,-0.75359157
55,4.1706158595,1.2608842805\H,-3.1575605672,2.8033392048,1.3056906862\H,-2.3515069422,2.6793689289,2.879
859866\H,-3.8517049897,3.6198943076,2.7238719677\H,-0.9492460055,3.5451290859,0.3868183663\H,-0.16750484
59,5.0276861974,0.9177254396\H,-0.1597645791,3.5973746977,1.9803468756\O,-3.9608402099,5.9801561479,1.456
4525713\O,-2.6244631457,5.5012432515,-0.2777472481\C,-4.7661432444,6.7556393455,0.5664297099\H,-5.5874948
162,7.1388714196,1.1690475584\H,-4.1777032631,7.5761585891,0.1487400328\H,-5.1386248903,6.1329235512,-0.2
493615751\\Version=ES64L-G09RevD.01\State=2-A\HF=-1037.6064323\S2=0.758244\S2-1=0.\S2A=0.750048\RMS
D=1.560e-09\RMSF=1.385e-05\ZeroPoint=0.393878\Thermal=0.4185881\Dipole=0.1773916,-0.4367488,1.1629636\P
G=C01 [X(C15H25O6)]\\@

Tri-rad (pro-m)

1\1\GINC-R456\Freq\UM062X\6-31+G(d,p)\C15H25O6(2)\ROOT\29-Jan-2014\0\\#N Geom=AllCheck Guess=TChec
k SCRF=Check Test GenChk UM062X/6-31+G(d,p) Freq\\MMA_trimer_rad.a0d3e2.freq\\0,2\C,2.5565942897,3.21037
85281,-1.6119540157\H,1.9482030565,3.6040034204,-2.4322295388\H,1.8935463605,2.7760323948,-0.8587902665\
H,3.1874963835,2.4035366103,-1.9904564947\C,3.4188740912,4.3352271098,-1.0312297253\C,2.5893204815,5.5596
513498,-0.5936991208\H,3.2530525986,6.2686024894,-0.0873130457\H,2.2384034728,6.0617175653,-1.5006367568\
C,1.3750781538,5.3278749234,0.3349963904\C,4.277500357,3.7603658813,0.0911500685\C,4.41786664,4.77706305
66,-2.1602029577\H,3.8039625392,5.1635594216,-2.9801862005\H,4.9352261685,3.8734098853,-2.5061596137\C,5.
4343505127,5.7997139758,-1.777079108\O,4.5802036892,2.5938843328,0.1962957279\O,4.7416142987,4.702664846
3,0.9319684573\C,5.5921017031,4.2237640299,1.9743085037\H,5.8747472063,5.1022612164,2.5521685338\H,5.054
662948,3.5052951002,2.5977707018\H,6.4747771076,3.7372065518,1.5520536033\C,6.745084782,5.4112646537,-1.1
773814174\H,7.5692477947,5.6450192719,-1.8635721095\H,6.9388258027,5.9700034855,-0.2558527421\H,6.773455
0422,4.3405240008,-0.9577707843\C,5.1450431865,7.1961700889,-2.0643378931\O,4.1235390178,7.6049150053,-2.
5934390031\O,6.1473869376,8.0235939101,-1.685512324\C,5.9199331568,9.4063693621,-1.951444771\H,6.8094054
432,9.9252740325,-1.5980017091\H,5.7768925744,9.5701121731,-3.0218483537\H,5.0322167374,9.755594867,-1.41
92234134\C,0.8347112619,6.7152683458,0.7419066558\C,0.2250057197,4.6305980721,-0.3872374574\C,1.71493602
34,4.530414464,1.5961507534\H,-0.0768736586,6.6174079754,1.3401082641\H,1.585835287,7.2338207409,1.345632
3735\H,0.6147294879,7.3238448787,-0.139061511\H,0.8325524672,4.4405921931,2.2339025259\H,2.0462224588,3.5
125993023,1.3654252851\H,2.5070564578,5.041776539,2.1498218528\O,-0.0297392586,5.1795132329,-1.588859694
4\O,-0.4339594489,3.7224595556,0.0637579621\C,-1.1126924854,4.5917410999,-2.3108954829\H,-1.1838762291,5.1
497465388,-3.2427754616\H,-0.9057864688,3.5364438058,-2.5057475365\H,-2.0391681482,4.6710767156,-1.738646
1506\\Version=ES64L-G09RevD.01\State=2-A\HF=-1037.6053868\S2=0.758255\S2-1=0.\S2A=0.750048\RMSD=2.02
7e-09\RMSF=1.092e-05\ZeroPoint=0.3940546\Thermal=0.418618\Dipole=0.8488094,1.0143341,0.0172587\PG=C01 [
X(C15H25O6)]\\@

Tri-rad (pro-r) Li+(Mon)$_2$

1\1\GINC-R453\Freq\UM062X\6-31+G(d,p)\C25H41Li1O10(1+,2)\ROOT\10-Nov-2013\0\\#M062X/6-31+G(d,p) INT
(grid=ultrafine) SCF=tight Freq=(noraman) maxdisk=3489660928\\MMA_trimer_rad_Li+.both.A1-11.MMA2.freq\\1,2
\C,0.0329482839,0.0228082631,0.013377391\C,0.0401954035,0.0539033455,1.5552962365\C,1.5259930409,0.014429
3138,2.0762257577\C,2.3087310119,-1.2096652143,1.7368427986\C,2.2429106942,-2.3203398922,2.6683098789\O,2
.9952318547,-3.3622419695,2.3209721311\C,2.979730924,-4.4854503778,3.2109061983\C,-0.5956569025,1.3247832
266,2.1283598015\C,-0.6177336788,-1.1664420416,2.1819707519\O,-0.4960437408,-2.2727785865,1.4608760051\C,-

1.0640198283,-3.4669228044,2.0210024426\O,-1.1308397745,-1.1645156159,3.2919661528\C,3.1207713718,-1.3325040129,0.493895063\O,1.5576911641,-2.3284926104,3.698655696\Li,-0.0029678409,-1.888745467,4.7535567788\O,-0.5839388411,-3.5161422667,5.4858281786\C,-0.295565381,-4.3832343318,6.3056162617\O,-1.0568556326,-5.448599173,6.485042713\C,-2.2454722235,-5.5362208284,5.6866703312\C,0.9199109341,-4.3257070518,7.1622596774\C,1.7316097138,-3.0660877806,7.051834466\C,1.2194267426,-5.3554953405,7.9601500238\O,0.2168958088,-0.3632903554,5.8077578638\C,0.4290093571,0.8433751375,5.7501738074\C,1.805880823,1.4016175997,5.6590572988\C,2.9121298244,0.3942656381,5.8006196\O,-0.5453940586,1.7336460466,5.7536053053\C,-1.8883868771,1.2155355598,5.7786364521\C,1.9834395097,2.7092663345,5.4456247423\H,0.7548052094,0.7711310519,-0.3329032081\C,-1.3060404866,0.294268851,-0.7125807183\H,0.3961637536,-0.9538065048,-0.3243320528\H,-0.4488015983,1.3785543648,3.2096398074\H,-0.1259450358,2.2019395584,1.6728467767\H,1.4901898396,0.1320108415,3.1655594773\H,2.0217929657,0.8972899025,1.6579330386\H,-0.9249955372,-4.2360140223,1.2640011952\H,-0.5461268675,-3.7278123962,2.9477268192\H,-2.1245308224,-3.3089493876,2.2275421251\H,2.7570238609,-2.1580952631,-0.1304088682\H,3.0892806507,-0.4118756727,-0.0900710978\H,4.1645843656,-1.5686918848,0.7307988408\H,3.6149075049,-5.2348140135,2.7446898304\H,3.3766153762,-4.1963780521,4.1862631177\H,1.9602681442,-4.8594262871,3.3287240306\H,2.6086021898,-3.1239270143,7.6988350194\H,2.0640766189,-2.8998125248,6.0211754013\H,1.1396852579,-2.1920413383,7.3420865394\H,2.1047238884,-5.327698 6241,8.5877199785\H,0.5926730599,-6.2386967722,8.0072344914\H,-2.7432848727,-6.4473784506,6.009046209\H,-2.8771350269,-4.6638268228,5.8598072206\H,-1.980783606,-5.5953013585,4.6290944748\H,-2.5327008295,2.0901021463,5.732979842\H,-2.0466939413,0.5611356983,4.9186318566\H,-2.0516001843,0.6624437594,6.7048560768\H,3.8828941851,0.8689249251,5.6508109814\H,2.8950805207,-0.0606900542,6.7962815176\H,2.7934152571,-0.4215510843,5.0788788726\H,2.9825423756,3.1257502349,5.3623060271\H,1.1414639198,3.3869916207,5.3577199091\H,-1.6705596425,1.3669181913,1.9343745581\C,-1.0786226216,0.0403483217,-2.2172771354\C,-2.4545231917,-0.5890033727,-0.2202273908\C,-1.7270268834,1.758658352,-0.5872157033\H,-3.3641047181,-0.3649398831,-0.7810516528\H,-2.1997728249,-1.6423960277,-0.3638204458\H,-2.6892730058,-0.4187762461,0.8365879044\H,-1.9755272493,0.2911016441,-2.7912284732\H,-0.2458482305,0.6378563075,-2.5967522934\H,-0.8559753675,-1.0184160871,-2.3811614367\O,-0.7248815926,2.6012746201,-0.8896002035\O,-2.8353922536,2.1371320282,-0.2924075316\C,-1.0646227931,3.9932851629,-0.8589209305\H,-0.1593948916,4.5244117412,-1.1456848983\H,-1.8743486173,4.1986209055,-1.5609049756\H,-1.3832790739,4.2795688948,0.1460998026\\Version=ES64L-G09RevD.01\State=2-A\HF=-1736.3869131\S2=0.75607\S2-1=0.\S2A=0.75003\RMSD=8.729e-10\RMSF=2.608e-06\ZeroPoint=0.6496967\Thermal=0.6945185\Dipole=1.3703293,-1.4701705,1.0645278\PG=C01 [X(C25H41Li1O10)]\\@

Tri-rad (pro-m) Li+(Mon)$_2$

1\1\GINC-R807\Freq\UM062X\6-31+G(d,p)\C25H41Li1O10(1+,2)\ROOT\10-Nov-2013\0\\#M062X/6-31+G(d,p) INT (grid=ultrafine) SCF=tight Freq=(noraman) maxdisk=3489660928\\MMA_trimer_rad_Li+.both.A1-4.MMA2.freq\\1,2\C,-2.7567024875,2.0733794799,-0.1483334534\C,-1.8725063015,0.8594891153,0.1462326804\C,-1.1953338366,1.0039172276,1.5585388908\C,-0.3172996477,2.1997247783,1.7324928629\C,1.0954603279,2.0659271675,1.4279671684\O,1.7982316757,3.1760737726,1.6455362252\C,3.2039009588,3.1046168995,1.3764937877\C,-2.6580632112,-0.4687641594,0.1819747824\C,-0.7057371345,0.7411315555,-0.82420429\O,-0.4297271024,1.8591815262,-1.4740577567\C,0.7111182915,1.8283962244,-2.3473561606\O,-0.0246082534,-0.2692163193,-0.9403708404\C,-0.8369669463,3.5023865817,2.237870936\O,1.6304502583,1.0320255161,1.0099907487\Li,1.7403455779,-0.5028443584,-0.1336954156\O,3.2433380352,-0.2280737811,-1.2291835071\C,4.4707342001,-0.2502707607,-1.1966430838\O,5.1970804903,0.0008576881,-2.2722590724\C,4.4844409558,0.2887664237,-3.4826873311\C,5.25127058,-0.5497047766,0.0343020694\C,4.4420532756,-0.9295895838,1.2423240545\C,6.5855847241,-0.4716192249,0.0086126585\O,1.4468528762,-2.2388922038,0.5625888267\C,0.3902300102,-2.6843404066,0.999286208\C,-0.0346771081,-2.4782928499,2.4114539707\C,0.9757757417,-1.7875643732,3.2836067372\O,-0.4494908983,-3.3794035637,0.2526897625\C,-0.0713003714,-3.5807836342,-1.1197087043\C,-1.2443720703,-2.8817406951,2.8131278541\H,-3.5778331365,2.1037170231,0.575223883\H,-3.1861760623,2.0269524208,-1.1522065205\H,-2.1940278367,3.0062919386,-0.0806742502\H,-1.9342428574,-1.2856592074,0.2813329171\H,-3.2685551584,-0.4688515419,1.0917008163\H,-0.6245476632,0.0881839385,1.7481542485\H,-2.0124167588,1.0513576682,2.286911174\H,0.731756612,2.8028540775,-2.8298582964\H,1.6201052071,1.6564696276,-1.7647235604\H,0.5940211211,1.0294690572,-3.0819611376\H,-0.6146663218,4.3160388922,1.5377457186\H,-1.9144975178,3.4593703512,2.4008876119\H,-0.3481372686,3.7734681011,3.1817437299\H,3.5863588569,4.1059130467,1.5595213765\H,3.6769287092,2.3832565222,2.0460936893\H,3.3746925118,2.8064376402,0.339523158\H,5.098574337,-1.1025630882,2.0965414034\H,3.72919496,-0.1395199012,1.5034931553\H,3.8630439533,-1.8401330203,1.0580912067\H,7.1674510427,-0.6842523315,0.8999774173\H,7.1218814474,-0.2001318154,-0.8934456952\H,5.249109928,0.4190805823,-4.2444888562\H,3.8218600447,-0.5410776894,-3.7332160374\H,3.9013690888,1.2042777765,-3.363044944\H,-0.8792565535,-4.1626812961,-1.5582138206\H,0.0335739522,-2.614177563,-1.6154195304\H,0.8696438053,-4.1311675325,-1.1661668734\H,0.5740155966,-1.6347168799,4.2864235882\H,1.8919044943,-2.3814846647,3.3588645035\H,1.2612661712,-0.8182984552,2.8588416266\H,-1.567863535,-2.7269151853,3.8379400483\H,-1.9303748651,-3.3769235159,2.1339061112\C,-3.5743789151,-0.8136005675,-1.0115001458\C,-4.0764544098,-2.2560960184,-0.7955466101\C,-4.8155792309,0.076708631,-1.0538128382\C,-2.8584514826,-0.721468455,-2.36015

89066\H,-4.7726045336,-2.5485447646,-1.587022571\H,-3.2243505914,-2.9439352772,-0.8147282112\H,-4.5835592847,-2.3561369831,0.1678495143\H,-3.5288993924,-1.029941096,-3.1648522168\H,-2.5427988034,0.3020889944,-2.5910568594\H,-1.9789736047,-1.3719398905,-2.358712765\O,-5.4184124598,0.1628893786,0.1435540305\O,-5.2429719984,0.6173106892,-2.0455007478\C,-6.6254857265,0.9363081964,0.166529635\H,-6.9885838558,0.8861092798,1.1908928568\H,-6.4146522239,1.9683517237,-0.1226796247\H,-7.3557374013,0.5144599175,-0.5257860098\\Version=ES64L-G09RevD.01\State=2-A\HF=-1736.3885497\S2=0.756221\S2-1=0.\S2A=0.750031\RMSD=2.786e-09\RMSF=5.382e-06\ZeroPoint=0.6498678\Thermal=0.69461\Dipole=2.1074474,0.4822498,0.7140693\PG=C01 [X(C25H41Li1O10)]\\@

Kinetic pathways

Di-rad Li+TS (rad-monC)

1\1\GINC-V1411\Freq\UM062X\6-31+G(d,p)\C10H17Li1O4(1+,2)\BXN501\22-Dec-2012\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk UM062X/6-31+G(d,p) Freq\\MMA_dimer_TS_Li+.A.freq\\1,2\C,-0.0010919855,0.0030702436,0.0045803677\H,-0.0562999739,-0.0258471684,1.0959371813\H,1.0623623365,0.0458420164,-0.2666052554\H,-0.4066876986,-0.9221297873,-0.4071475526\C,-0.7022472093,1.2164716592,-0.5230339873\C,-0.4878233769,2.5204517778,0.1810212962\H,-1.1034539607,3.320821947,-0.2314345153\H,-0.6824604054,2.4220400989,1.2523982179\H,0.5631300252,2.8203049039,0.0724090069\C,-1.0199971755,1.2807832285,-1.9472117228\C,-2.8296054842,0.8471897045,0.0576782453\H,-3.1189083113,1.8557304603,-0.2236428635\H,-2.4622833682,0.712668694,1.0708786918\C,-3.3615584157,-0.2324514759,-0.5994395868\O,-1.4714848206,2.2905248002,-2.5111505977\O,-0.846510836,0.1366267819,-2.591439839\C,-1.1328087056,0.1141136499,-3.9977994433\H,-0.8153819158,-0.8673223621,-4.3415010738\H,-2.2062228145,0.243060109,-4.1636681107\H,-0.5765814847,0.9018894889,-4.5072792404\C,-3.2190459292,-1.6448814856,-0.1188487391\H,-2.7102674126,-2.2671580197,-0.8631363484\H,-2.6527726181,-1.6758734511,0.8132766246\H,-4.2003729298,-2.0973857152,0.0530673318\C,-4.1047176498,0.0114202628,-1.8471944324\O,-4.1531384339,1.0946003089,-2.4504140988\O,-4.7448601236,-1.0495947393,-2.288454793\C,-5.5436318986,-0.9031929751,-3.4764038776\H,-5.9980066287,-1.8772023195,-3.6369550056\H,-6.3045570134,-0.1382956195,-3.3176918436\H,-4.9083000252,-0.6292546248,-4.3202791743\Li,-3.2105689353,2.5676440728,-2.9045545266\\Version=EM64L-G09RevA.02\State=2-A\HF=-699.279032\S2=0.778298\S2-1=0.\S2A=0.750208\RMSD=2.360e-09\RMSF=2.763e-06\ZeroPoint=0.2640682\Thermal=0.2819867\Dipole=-0.5493454,0.8978213,-0.8417816\PG=C01 [X(C10H17Li1O4)]\\@

Di-rad Li+TS (monC)

1\1\GINC-V1397\Freq\UM062X\6-31+G(d,p)\C10H17Li1O4(1+,2)\BXN501\22-Feb-2013\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk UM062X/6-31+G(d,p) Freq\\MMA_dimer_TS_Li+.monoC.2.freq\\1,2\C,0.002638736,0.0142878782,0.0113519639\H,-0.0485118801,-0.0066238715,1.1032509998\H,1.0636739306,0.0596768876,-0.270946399\H,-0.3977369465,-0.9172586316,-0.3933833895\C,-0.7063100862,1.2126146543,-0.5296578025\C,-0.5057486808,2.5327868008,0.1409716817\H,-1.155869607,3.3022415774,-0.2782496205\H,-0.6579036158,2.4566799324,1.2212795399\H,0.5320515149,2.8595798936,-0.0146708948\C,-1.0560341946,1.2625691806,-1.9667714071\C,-2.8699566242,0.8515082688,0.0919433071\H,-3.1062308032,1.8235808894,-0.3318851364\H,-2.5495867395,0.8171410994,1.1284431349\C,-3.330869234,-0.2824651641,-0.5157515299\O,-1.5421572871,2.228588466,-2.5181354828\O,-0.8251647482,0.0968622268,-2.603743059\C,-1.047195596,0.1296056512,-4.0193243698\H,-0.7879211113,-0.8635825095,-4.3814121237\H,-2.0896197583,0.3722581981,-4.2403546137\H,-0.4089512307,0.8842504772,-4.4817560311\C,-3.9417101215,-0.2836469175,-1.8900246035\H,-5.0048278442,-0.5708551876,-1.8637004696\H,-3.9039669635,0.7140330563,-2.3339713349\H,-3.3863306486,-0.9454361051,-2.5735658348\C,-3.2154876745,-1.5780539839,0.1378729395\O,-3.6543926988,-2.6277412074,-0.3809421535\O,-2.6345649964,-1.5938435131,1.3151416018\C,-2.5292163115,-2.8623770057,1.9898191357\H,-2.0320475316,-2.6430826,2.9309717792\H,-3.5244083029,-3.2732565891,2.1626240459\H,-1.9373017329,-3.5528107837,1.3877531101\Li,-4.4895453386,-2.9222218893,-1.904606221\\Version=EM64L-G09RevA.02\State=2-A\HF=-699.2403487\S2=0.774907\S2-1=0.\S2A=0.750222\RMSD=1.463e-09\RMSF=1.428e-06\ZeroPoint=0.2628709\Thermal=0.2813678\Dipole=-2.2729819,-3.3458655,-0.5505126\PG=C01 [X(C10H17Li1O4)]\\@

Di-rad Li+TS (radC)

1\1\GINC-V1362\Freq\UM062X\6-31+G(d,p)\C10H17Li1O4(1+,2)\BXN501\23-Feb-2013\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk UM062X/6-31+G(d,p) Freq\\MMA_dimer_TS_Li+.radC.2.freq\\1,2\C,0.005804298,-0.005538013,0.0007715174\H,-0.0528061737,-0.0471448687,1.0905765702\H,1.0707435345,0.0426906143,-0.2643426867\H,-0.406722196,-0.9356430796,-0.4002282865\C,-0.7105768905,1.2088228178,-0.5141145853\C,-0.544527224,2.4879900602,0.2481656341\H,-1.1764794624,3.2852034539,-0.1440513532\H,-0.7865830299,2.3380364607,1.3030835617\H,0.5008068051,2.8186972365,0.1827407707\C,-0.9586659468,1.2641176301,-1.9358441648\C,-2.8006853999,0.5911510902,-0.0157432328\H,-2.4556988912,0.405539752,0.9974275952\H,-2.7863397064,-0.2398817252,

-0.7166059232\C,-3.6523351557,1.6403609698,-0.2314292547\O,-0.8294584028,0.2831480619,-2.7119427046\O,-1.3940757329,2.424597657,-2.3882148146\C,-1.7132441813,2.5344117126,-3.7821986009\H,-2.0608585321,3.5558974563,-3.9168987713\H,-0.8221517244,2.3538995435,-4.3857735042\H,-2.4991694923,1.8241137123,-4.0460643136\C,-4.3878625354,1.8720385327,-1.5121407117\H,-4.1572982125,2.8604505316,-1.9234613367\H,-4.1373349955,1.1029922718,-2.2479030963\H,-5.4693396196,1.8522521511,-1.3421849122\C,-3.8202886224,2.606829824,0.8938231523\O,-3.2201887497,2.534512797,1.9450745135\O,-4.7101033969,3.5590414917,0.6057648644\C,-4.9544477045,4.5130215844,1.6510154883\H,-5.7048682828,5.193256214,1.2554762284\H,-5.3211777038,4.0013490442,2.5421704826\H,-4.032796915,5.0449744877,1.8927166752\Li,-0.2869073722,-1.1754635914,-3.4417874675\\Version=EM64L-G09RevA.02\State=2-A\HF=-699.2393956\S2=0.775835\S2-1=0.\S2A=0.75019\RMSD=4.862e-09\RMSF=6.312e-07\ZeroPoint=0.2630873\Thermal=0.2816927\Dipole=2.3523906,-3.2840236,-3.9353153\PG=C01 [X(C10H17Li1O4)]\\@

Di-rad Li+ (Mon) (rad-monC)

1\1\GINC-V1299\Freq\UM062X\6-31+G(d,p)\C15H25Li1O6(1+,2)\BXN501\24-Apr-2013\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) SCF=tight Freq=(noraman) maxdisk=671088640\\MMA_dimer_rad_mono_Li+.1.MMA.freq\\1,2\H,-4.0673874845,-2.5536655424,0.2471863748\C,-3.7937485333,-1.9196268258,-0.6000622194\H,-4.5963465588,-1.1954971518,-0.7528905008\H,-3.7186069899,-2.5525933606,-1.4892291256\C,-2.4499251533,-1.231379414,-0.3505076382\H,-1.5976248224,-3.005016808,0.563369817\H,-1.2044926796,-2.8141760446,-1.1515093201\H,-0.3850651917,-1.8153007733,0.0762082701\C,-1.3352535411,-2.2748461837,-0.2078968557\C,-2.4616467885,-0.3657106705,0.907526261\O,-1.4509253558,0.0455079756,1.445779797\O,-3.6840393368,-0.0651396458,1.3324300254\C,-3.7604743286,0.7802161671,2.4873841685\H,-3.2534977334,0.3090737982,3.3308058463\H,-4.8216315947,0.9031103594,2.6907215922\H,-3.2916440453,1.7430783759,2.2749830742\C,-2.1635038674,-0.2687726006,-1.5556251167\H,-2.9867944255,0.4492150319,-1.6218809963\H,-2.1805838514,-0.8886885521,-2.4586714469\C,-0.8578858353,0.4482286467,-1.4742330808\C,-0.7587110082,1.7029593236,-0.7572443109\O,-1.9166015648,2.2538160308,-0.4340525422\C,-1.8651037289,3.4572745314,0.3468557495\H,-1.3880904681,3.2471997693,1.3068260923\H,-1.308269266,4.2281254192,-0.1873753188\H,-2.9016980609,3.7570633382,0.4826757133\O,0.3217525049,2.2466064828,-0.4661971595\C,0.3963560534,-0.122703953,-2.0448592906\H,1.0149838593,-0.5902953939,-1.2637780613\H,0.1714633514,-0.8970908073,-2.7802945692\H,1.0059619229,0.6518848482,-2.5221466249\H,0.9585114819,0.0319739172,0.9958021501\C,1.7138471847,-0.4155778726,1.6542561065\H,1.1645479999,-1.0610788432,2.3409490709\C,2.7484116556,-1.2022160221,0.8981877714\H,2.2776235549,-3.1149784788,1.6476082596\H,3.6763821767,-3.0457379326,0.4248719465\C,2.9119937388,-2.5264025544,0.9921291545\C,3.6201306485,-0.4177899426,-0.0144192779\O,4.6387439969,-1.0639259481,-0.5269100457\C,5.5006944806,-0.3383705802,-1.4244452079\H,4.9310565832,0.0005628569,-2.2906665317\H,5.9368187992,0.515670198,-0.9054191431\H,6.2686617205,-1.0489865648,-1.7178040039\O,3.4037147922,0.7698334722,-0.2803544535\H,2.1796844811,0.3825413407,2.2435280498\Li,2.0457452277,1.9535705838,-0.1187944491\\Version=EM64L-G09RevA.02\State=2-A\HF=-1044.9950579\S2=0.755525\S2-1=0.\S2A=0.750026\RMSD=4.141e-09\RMSF=4.181e-06\ZeroPoint=0.3935135\Thermal=0.4209597\Dipole=1.6485239,0.8217178,-0.3350227\\PG=C01 [X(C15H25Li1O6)]\\@

Tri-rad Li+TS (rad-monC)gas

1\1\GINC-V1277\Freq\UM062X\6-31+G(d,p)\C15H25Li1O6(1+,2)\BXN501\12-Apr-2013\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk UM062X/6-31+G(d,p) Freq\\MMA_trimer_TS_Li+.2.freq\\1,2\C,-0.0736158728,-0.0330395539,0.0506129489\H,-0.0336963605,0.0013581291,1.1413504759\H,0.9579660119,-0.1763813296,-0.3037492519\H,-0.6493448664,-0.8972790596,-0.2835463023\C,-0.6270831937,1.2484752631,-0.4949884095\C,-0.194072883,2.5593630818,0.1010809384\H,-0.7393534611,3.3773790476,-0.379215538\H,-0.4190881001,2.5678440691,1.1727050653\C,1.3227653643,2.85288824,-0.0541919302\C,-1.0551733035,1.2772520418,-1.8940161435\C,-2.7136968576,1.2059857396,0.2848232347\H,-2.903892695,2.2204735785,-0.0542007635\H,-2.2731769054,1.1000072089,1.2717847839\C,-3.433997977,0.1580990977,-0.2316498067\O,-1.4400526238,2.3002256691,-2.4855116225\O,-1.0624610196,0.0899875509,-2.4815430246\C,-1.4712064236,0.0302649483,-3.8556480294\H,-1.2983195684,-0.9979284783,-4.1641026552\H,-2.5334168686,0.2763041067,-3.9419976446\H,-0.8761718233,0.7204245844,-4.4550966689\C,-3.4248741238,-1.219245165,0.3594533661\H,-3.0796418984,-1.9615733461,-0.3683309675\H,-2.7750412311,-1.2542854971,1.2351010327\H,-4.4337635475,-1.5182838137,0.6601808185\C,-4.2531756939,0.4003703385,-1.4291796365\O,-4.231637097,1.4355290583,-2.113780746\O,-5.0500136424,-0.6029649789,-1.7294518053\C,-5.9283035213,-0.4440505106,-2.8575546225\H,-6.5049130442,-1.3640803606,-2.9027718514\H,-6.5786779322,0.4172999704,-2.7012018944\H,-5.3430727292,-0.3096251919,-3.7687773317\C,1.8016108987,2.6490241598,-1.4946811212\C,1.5698314988,4.3126523819,0.3744424408\C,2.0945430268,1.9940415038,0.9485770837\Li,-3.1696905114,2.7535965918,-2.7281669291\H,2.6392352647,4.5402273448,0.3563656513\H,1.0655080801,4.9920019798,-0.3195626433\H,1.1914658324,4.4947168809,1.3842663904\H,2.8406195612,2.9642243479,-1.6026737881\H,1.7469869041,1.5994535974,-1.8055930675\H,1.1834994416,3.2461056993,-2.1728054204\O,1.6516719443,1.6425161668,2.0193960864\O,3.3360860625,1.7243099517,0.5426786263\C,4.157328604,1.0147666422,1.4835193013\H,5.1236850904,0.8996031682,0.9983056317\H,4.248943325,1.5898163443,2.4061700114\H,3.714601994,0.0425028784,1.7068714738\\Version=EM64L-G09RevA.02

\State=2-A\HF=-1044.9717011\S2=0.778263\S2-1=0.\S2A=0.750206\RMSD=5.191e-09\RMSF=1.906e-06\ZeroPoint=0.3939282\Thermal=0.4198375\Dipole=-2.4832058,0.1570035,-2.2971547\PG=C01 [X(C15H25Li1O6)]\\@

Tri-rad Li+TS (rad-monC)sol

1\1\GINC-V1405\Freq\UM062X\6-31+G(d,p)\C15H25Li1O6(1+,2)\BXN501\05-May-2013\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk UM062X/6-31+G(d,p) Freq\\MMA_trimer_TS_Li+.A1.8.freq\\1,2\C,-0.0791073236,-0.08874407,0.0721231188\H,-0.1081167129,-0.0791451419,1.1642793184\H,0.9711856629,-0.1067322471,-0.2446649233\H,-0.536218776,-1.0099260741,-0.2961584085\C,-0.7364957132,1.1326268052,-0.4916424665\C,-0.6287571779,2.4584188388,0.2107739681\H,-1.3873256821,3.1355637022,-0.1915802334\H,-0.848602119,2.3086648545,1.2753745699\C,0.7461992248,3.205464673,0.1541349388\C,-0.9366408729,1.1365855428,-1.9412547754\C,-2.8645222333,0.6001092651,-0.0838074233\H,-2.6283939611,0.6722159888,0.9740030578\H,-2.739590663,-0.377422051,-0.5398268737\C,-3.738528498,1.5046636841,-0.6333820669\O,-0.9182772667,0.1150641666,-2.6461889913\O,-1.2061069613,2.3336670268,-2.4397179366\C,-1.3892923161,2.4615477003,-3.8566322948\H,-1.291571209,3.5247064167,-4.0652113688\H,-0.6291652157,1.8902822017,-4.390704424\H,-2.3872319145,2.1083225625,-4.1328903705\C,-4.1796019957,2.7585391495,0.0590177949\H,-5.2663304238,2.7682912106,0.1880093761\H,-3.711571205,2.8371195091,1.0415617512\H,-3.9231672333,3.6475180575,-0.5273686757\C,-4.2602153175,1.227716517,-1.9803643994\O,-3.861510607,0.3216870422,-2.7296825316\O,-5.2275182969,2.0424552244,-2.3442286011\C,-5.8435601783,1.8202734266,-3.6250032846\H,-6.620929207,2.5756359152,-3.7031924633\H,-5.1058446551,1.9422186327,-4.4198126044\H,-6.2690519161,0.8167630078,-3.6612340876\C,0.503232055,4.6464176468,0.6092827171\C,1.784015646,2.5404045873,1.0717902426\C,1.2732421936,3.2280815806,-1.2783642476\Li,-2.4372255516,-0.6499007369,-3.2594344729\H,2.7237479536,3.0997319456,1.0444641279\H,1.4189225563,2.5521537892,2.1035464868\H,2.0012761826,1.5111400963,0.7857911762\H,1.4418090154,5.2053865368,0.6288804001\H,-0.1789758653,5.1652977962,-0.0677088955\H,0.0786671988,4.6491454882,1.617816076\O,1.684269288,2.002344575,-1.6756973786\O,1.3286490614,4.1946702178,-1.9950209552\C,2.2603358916,1.9394108288,-2.9862026297\H,2.4540047363,0.8852779727,-3.1755215909\H,1.570102318,2.35216769,-3.7251336901\H,3.1872659735,2.5148248011,-3.0139098304\\Version=EM64L-G09RevA.02\State=2-A\HF=-1044.9697118\S2=0.778424\S2-1=0.\S2A=0.750202\RMSD=2.617e-09\RMSF=6.311e-06\ZeroPoint=0.3936763\Thermal=0.4196382\Dipole=-2.0602772,-2.2595415,-1.2446863\PG=C01 [X(C15H25Li1O6)]\\@

Tri-rad Li+TS (monC) Mon

1\1\GINC-R715\Freq\UM062X\6-31+G(d,p)\C20H33Li1O8(1+,2)\ROOT\18-Jan-2014\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) SCF=tight Freq=(noraman)maxdisk=1342177280\\MMA_trimer_TS_monoC_Li+.5.MMA.freq\\1,2\C,-3.9423003097,-0.5341918203,0.1180416863\C,-2.9330306534,0.2461606294,-0.7781048629\H,-3.3236641127,1.2596250234,-0.9048828589\H,-2.9244782101,-0.2415394565,-1.7592674754\C,-1.5314738904,0.3022420865,-0.2375046766\H,-1.1544873863,-1.5388934399,0.7802987816\H,-0.8782874497,-1.6093008823,-0.9668138282\H,0.28927914,-0.7823761708,0.1117476863\C,-0.7672425883,-0.9754089387,-0.08104704\C,-1.1367647296,1.3904013304,0.6821471009\O,-0.0785518198,1.4130095619,1.2902515513\O,-2.0348367948,2.3820593921,0.7414999354\C,-1.7462741299,3.4316544341,1.6684518279\H,-1.6764367988,3.027697164,2.6805642118\H,-2.5756378835,4.1312351449,1.5887949535\H,-0.8045627318,3.9164885833,1.4083429144\C,-0.4845349744,1.2639998099,-1.9891022776\H,-1.0596376913,2.1777023103,-1.8723969295\H,-0.9012799388,0.495694585,-2.6339414186\C,0.8561077772,1.2456021298,-1.7129016087\C,1.4719005939,2.3575754435,-0.9875624995\O,0.7131656517,3.423780992,-0.8178780805\C,1.3026570495,4.5246266665,-0.1083092682\H,1.5454225332,4.2158281559,0.9108310233\H,2.2044185703,4.8600667262,-0.6221580165\H,0.5474789621,5.3074585707,-0.1114114472\O,2.6430566948,2.3319161214,-0.5777451164\C,1.7527277602,0.0897245782,-2.0490892043\H,2.140282128,-0.4027248151,-1.1472475175\H,1.2097458747,-0.6609232874,-2.625810749\H,2.6145158779,0.4188211355,-2.6406250175\H,2.1027059988,0.3110041679,1.1137316528\C,2.4977811731,-0.3543165557,1.8920843353\H,1.6575595534,-0.5574115676,2.5574121973\C,3.0554564093,-1.6337237492,1.3331048079\H,1.6541121531,-2.9643620513,2.1746333118\H,2.9822407838,-3.7398900734,1.1294220501\C,2.5378414153,-2.8469324087,1.5549015917\C,4.2574921724,-1.4942800687,0.4708936426\O,4.8683869634,-2.6108250929,0.1565783604\C,6.031249013,-2.5137578717,-0.6876745839\H,5.7557748993,-2.0749974513,-1.647544157\H,6.7897526686,-1.9006984224,-0.2000044185\H,6.3783923198,-3.5359177306,-0.8124051849\O,4.6623637632,-0.3973930093,0.0696277947\H,3.2586358535,0.1891287635,2.463851099\Li,3.9895912526,1.2799282434,-0.0650052014\C,-3.6076728074,-2.0240884753,0.1225598103\C,-3.9473457593,-0.0214512019,1.5579628962\C,-5.3415740653,-0.3774019486,-0.5043031856\H,-4.6955403205,-0.5564770156,2.1466452352\H,-2.9814864633,-0.1759897053,2.0505490259\H,-4.180581893,1.0465235865,1.5680255939\H,-6.0770626917,-0.9666268012,0.0514138501\H,-5.6459363305,0.6725052231,-0.4605015715\H,-5.3509562025,-0.7044890098,-1.5468550929\O,-3.5050327199,-2.5225754256,-1.1215977798\O,-3.4645095608,-2.7014895662,1.1127075319\C,-3.2516644402,-3.9301709546,-1.200276969\H,-3.2328817637,-4.1681755127,-2.261785802\H,-2.2937412559,-4.1664394179,-0.7305783155\H,-4.042452639,-4.4843316609,-0.6922023047\\Version=ES64L-G09RevD.01\State=2-A\HF=-1390.6462694\S2=0.776986\S2-1=0.\S2A=0.750208\RMSD=3.550e-09\RMSF=9.310e-07\ZeroPoint=0.5198666\Thermal=0.5556081\Dipole=3.4419385,0.7875425,-0.8708857\PG=C01 [X(C20H33Li1O8)]\\@

Tri-rad Li+TS (radC)

1\1\GINC-V1456\Freq\UM062X\6-31+G(d,p)\C15H25Li1O6(1+,2)\BXN501\03-May-2013\0\\#M062X/6-31+G(d,p) I
NT(grid=ultrafine) SCF=tight Freq=(noraman) maxdisk=402653184\\MMA_trimer_TS_radC_Li+.A1.8.freq\\1,2\C,0.0
128280666,0.0211154748,0.0999931705\H,-0.0298633213,0.0186125567,1.1925552101\H,1.0641481974,0.077268602
9,-0.196184395\H,-0.403685588,-0.9197716484,-0.2705246604\C,-0.7397330185,1.2455770914,-0.4771860444\C,-0.6
716794651,1.1267674726,-2.0261434692\C,-2.1595000991,1.0931418528,0.0400734516\O,-2.9908816894,0.3206886
213,-0.4409548556\O,-2.4160753658,1.7876741401,1.1205172596\C,-3.7006044636,1.6001707194,1.7483020571\H,-
3.6855044098,2.2425414889,2.624601105\H,-3.8219700408,0.554001392,2.030766792\H,-4.493309851,1.897945574
4,1.0611400489\C,-0.0782659874,2.5219745273,0.0559638971\H,0.0509313505,2.4603606714,1.1380465126\H,0.910
3854665,2.6332562929,-0.3982571332\H,-0.6622263226,3.4183489371,-0.155871458\C,-1.2909612447,2.1904144963
,-2.9047711602\H,0.4001195468,1.1060068504,-2.2525472845\H,-1.0601637927,0.1435778575,-2.3176544277\C,-2.6
742436415,2.0152831098,-3.3358590645\O,-3.3086751394,0.9444985941,-3.2905116181\Li,-3.5574431731,-0.291391
1395,-2.0342169669\O,-3.2020153737,3.0917458964,-3.8962029721\C,-4.5190535485,2.9646434351,-4.4574594099\
H,-4.522904818,2.1942565714,-5.2299598689\H,-4.7447488184,3.9400282127,-4.8808787661\H,-5.2359134387,2.70
90945687,-3.6757140309\C,-0.7499643651,3.5946068345,-2.8749285082\H,-1.2419190767,4.1941700758,-2.1011497
317\H,0.3238122531,3.5842037834,-2.6672284343\H,-0.917664797,4.0992265548,-3.827918117\C,-0.6026334097,1.4
947057917,-4.8689225357\C,0.7628211817,1.6684958937,-4.8910192962\H,-1.2209964693,2.2041090969,-5.4117798
514\H,-1.0001149129,0.4922151093,-4.7271531794\C,1.7480832055,0.6396707737,-4.4401360521\H,1.2491073514,-
0.274462172,-4.1124480061\H,2.4328714584,0.3940527224,-5.2592441238\H,2.3822197145,1.0280335351,-3.634682
9366\C,1.3596811742,2.9591901674,-5.3368927626\O,2.5364464195,3.2133407444,-5.2126527509\O,0.470314974,3.
7996208889,-5.8866735963\C,1.013696772,5.0490410334,-6.3379754823\H,1.4448826586,5.5952963501,-5.4966842
025\H,0.1767361949,5.593817604,-6.7690484579\H,1.7883058234,4.8708160368,-7.0853509495\\Version=EM64L-G
09RevA.02\State=2-A\HF=-1044.9654389\S2=0.77838\S2-1=0.\S2A=0.750212\RMSD=4.307e-09\RMSF=1.239e-06\Z
eroPoint=0.3941943\Thermal=0.4201892\Dipole=-2.9441339,-1.5171078,1.3945826\PG=C01 [X(C15H25Li1O6)]\\