Electronic Supplementary Material (ESI) for Nanoscale.

Electronic Supplementary Information:

Dye···TiO_2 Interfacial Structure of Dye-Sensitised Solar Cell Working Electrodes Buried under a Solution of I^-/I_3^- Redox Electrolyte

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1 Substrate Characterisation

The silicon-TiO_2 substrate surface was examined using atomic force microscopy (AFM) in tapping mode (**Figure S1**). Surface roughness was calculated as R_a = 1.2 Å; and R_q = 1.6 Å

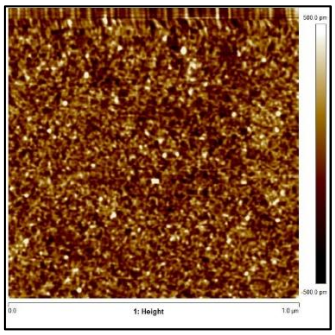


Figure S1 AFM image of freshly deposited TiO_2 thin-film on silicon wafer substrate.

The amorphous nature of the film was confirmed using Bragg-Brentano X-ray diffraction (**Figure S2**)

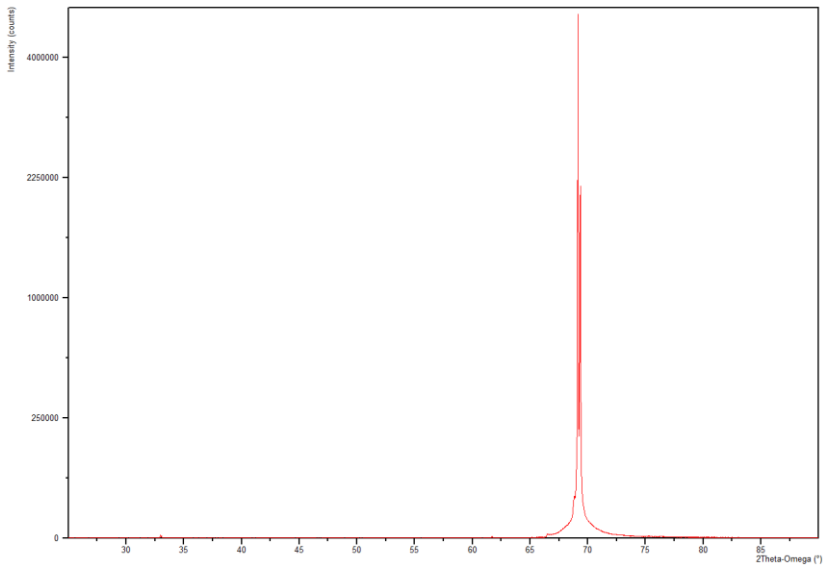


Figure S2 XRD pattern of the TiO_2 thin-film, the plot is dominated by the silicon 400 peak 69°, with a small peak at 33° corresponding to the Si(200) reflection. The absence of any discernible TiO_2 peaks confirms the films amorphous nature.

2 Reflectometry

2.1 Molecular Dimensions

The figures below pictorially represent the molecular dimensions taken for the **MK-2** (**Figure S3**) and **MK-44** dye molecules (**Figure S4**), as used in calculations for the XRR and NR studies.

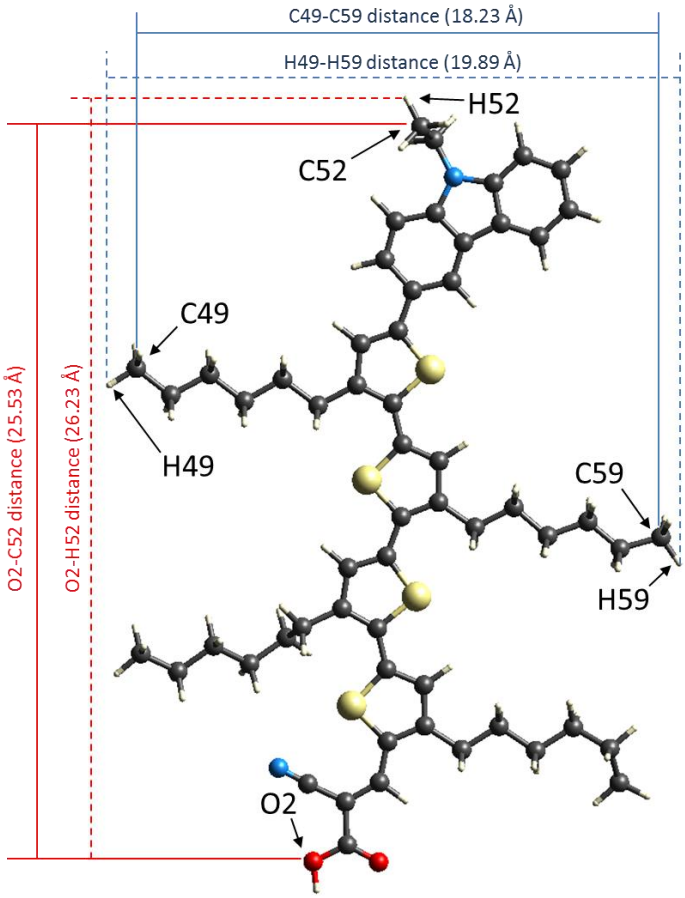


Figure S3 Molecular structure of the **MK-2** molecule, indicating labelled atoms and dimensions as used for calculations in the XRR study (solid lines); and NR study (dashed lines), inclusive of hydrogens. Values taken as the molecular height are shown in red, and molecular width in blue. The **MK-2** structure is taken from crystallographic data[1] and imaged using CrystalExplorer 3.0.[2]

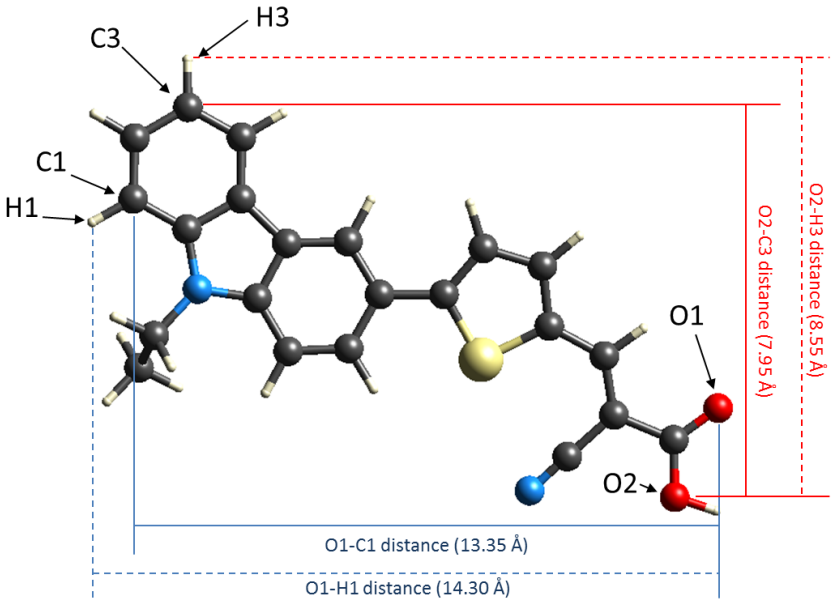


Figure S4 Molecular structure of the **MK-44** molecule, indicating labelled atoms and dimensions as used for calculations in the XRR study (solid lines); and NR study (dashed lines), inclusive of hydrogens. Values taken as the molecular height are shown in red, and molecular width in blue. The **MK-44** structure is taken from crystallographic data[1] and imaged using CrytsalExplorer 3.0.[2]

2.2 X-Ray Reflectivity and SLD profiles for MK-2 and MK-44 dyes

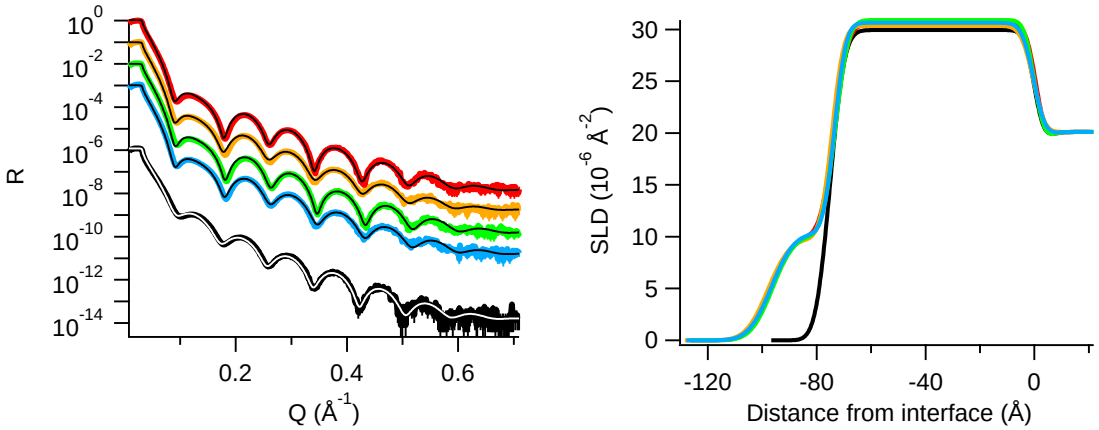


Figure S5 a) Reflectivity profile for TiO_2 substrates sensitised with the **MK-2** dye (red, orange, green, blue). The corresponding fitted models are represented by the overlaying black lines. The substrate prior to sensitisation is shown as the black trace, with corresponding model in white and indicated the surface was free from contamination (*e.g.* water). b) Corresponding SLD profile, offset to place the silicon interface at 0 Å

Table S1 Structural data as observed from XRR model refinements for **MK-2** sensitised TiO_2 substrates

	Dye			**TiO_2**		
Sample	**t /Å**	**SLD (x10^{-6}) /Å^{-2}**	**R /Å**	**t /Å**	**SLD (x10^{-6}) /Å^{-2}**	**R /Å**
1	23.0	10.1	6.2	74.2	30.5	4.0
2	23.5	9.8	6.4	74.3	30.3	3.4
3	23.1	10.1	6.2	73.2	30.9	3.8
4	23.2	10.3	6.6	73.4	30.6	3.3

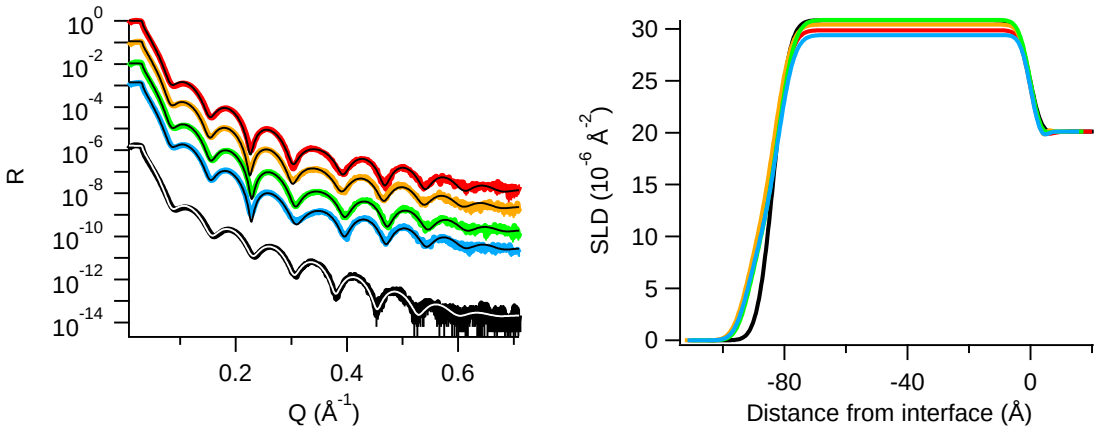


Figure S6 a) Reflectivity profile for TiO_2 substrates sensitised with the **MK-44** dye (red, orange, green, blue). The corresponding fitted models are represented by the overlaying black lines. The substrate prior to sensitisation is shown as the black trace, with corresponding model in white and indicated the surface was free from contamination (*e.g.* water). b) Corresponding SLD profile, offset to place the silicon interface at 0 Å

Table S2 Structural data as observed from XRR model refinements for **MK-44**-sensitised TiO_2 substrates

	Dye			**TiO_2**		
Sample	**t /Å**	**SLD (x10^{-6}) /Å^{-2}**	**R /Å**	**t /Å**	**SLD (x10^{-6}) /Å^{-2}**	**R /Å**
1	9.6	9.6	3.5	82.7	29.9	4.1
2	9.5	9.6	3.7	83.1	30.4	4.2
3	9.6	9.2	3.5	82.0	30.9	4.2
4	9.9	9.8	3.7	82.2	31.1	4.2

2.3 Molecular Tilt

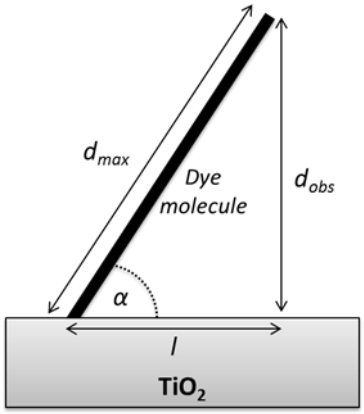
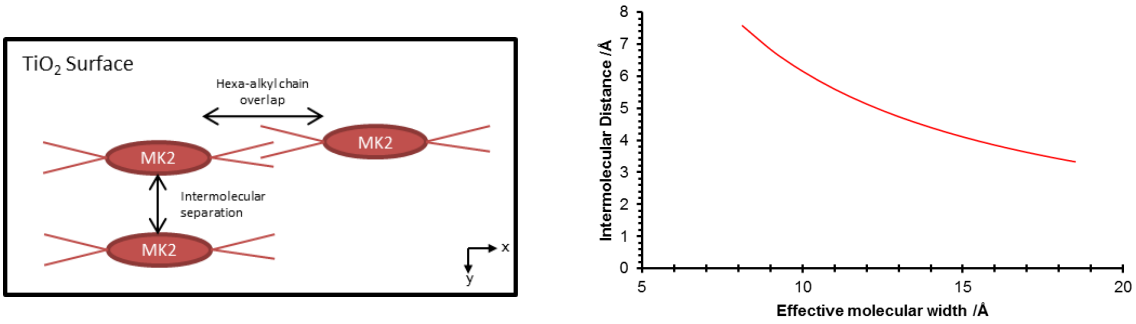


Figure S7 Diagrammatic representation of the simple trigonometric relation of the dye tilt angle (α) to d_{max} (the maximum possible dye thickness with the dye orientated perpendicular to the surface) and d_{obs} (the observed dye-layer thickness).

2.4 Justifying the MK-2 intermolecular distance



a **b**

Figure S8 (a) Interdigitation model of alkyl groups between **MK-2** molecules where their (b) intermolecular separation has an inverse relationship with the effective molecular width of **MK-2**.

It is not possible to offer an absolute value of intermolecular distance for **MK-2** due to its dependency on the overlap of hexa-alkyl chains on adjacent **MK-2** molecules, which is not directly measureable using XRR. **Figure S8(a)** shows a top-down view of a simplified **MK-2**-sensitised surface, indicating the two types of intermolecular overlap: intermolecular separation parallel to surface plane (here drawn stacking along the y-axis); and hexa-alkyl chain inter-digitation (here drawn along the x-axis). However, for the observed area per molecule (APM) of 61.6 ± 1.0 $Å^2$ and tilt angle (α) of 65.1 ± 1.1°, the interdependence between the intermolecular overlap and hexa-alkyl chain inter-digitation can be visualised, as shown in **FigureS8(b)**. It was therefore deemed more appropriate to present a range of overlap values, with the proviso that multiple overlapping states could co-exist on the TiO_2 surface.

3 Suitability of Neutron Reflectometry (NR)

3.1 The effect of fitting the dye layer to the neutron reflectometry data

Figure S9 below shows that fitting the dye layer to the data makes a large impact, *vis a vis* the Figure 5b in the article showed an excellent fit between the data and the three-layer model which includes the dye layer. Given the fit to the data is so good, they are represented in **Figure S9** by a single coloured line for the neutron reflectometry measurements on each solution. **Figure S9** also shows black lines that demonstrate the impact of including the dye layer on the fit to the data. The black lines are the fits presented in Fig. 5b of the paper, but with the dye layer removed. The difference between the black lines and coloured lines therefore demonstrates the effective contribution of the dye layer to the data, which **Figure S9** shows is quite marked. The suitability of neutron reflectometry to model dye layers in DSCs is thus readily justified.

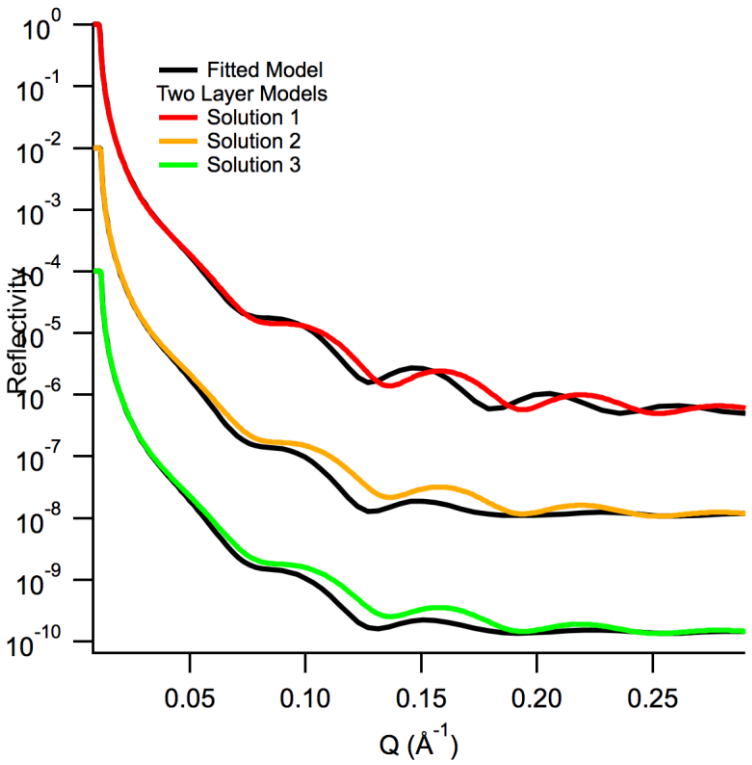


Figure S9. The coloured lines are the best fits shown in Figure 5b of the article; data points hidden for clarity. The black lines in each case represent the fit with the dye layer removed.

3.2 Simulated reflectivity and scattering length density profiles

One limitation of NR, when compared to XRR, is the range of Q accessible during experiments. With a good quality sample, typical lab-based XRR can reach a Q_{max} of 0.7-0.8 $Å^{-1}$, whereas NR is restrained by the flux of the neutron source and the higher level of background noise associated with a multiple beam-line environment. As such, a maximum Q of ~0.3 Å was achieved in this work.

Despite this limitation, the lower Q ranges should still be sufficiently sensitive to detect changes in dye thickness and SLD, as demonstrated in **Figure S10** and **Figure S11**.

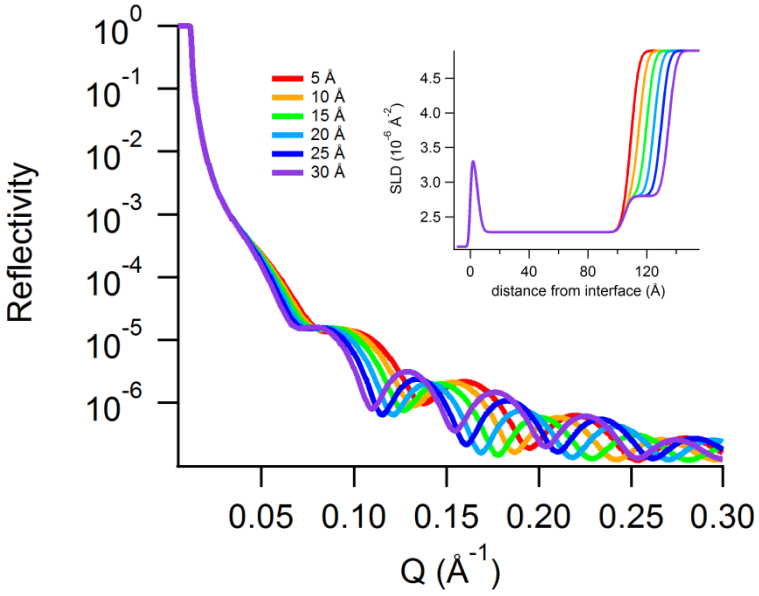


Figure S10 Simulated Reflectivity and (inset) SLD profiles for a dye layer of varying thickness, but fixed SLD (2.8×10^{-6} $Å^{-2}$) and roughness (4 Å). All other parameters were fixed at the calculated values highlighted in **Table 2** of the main manuscript.

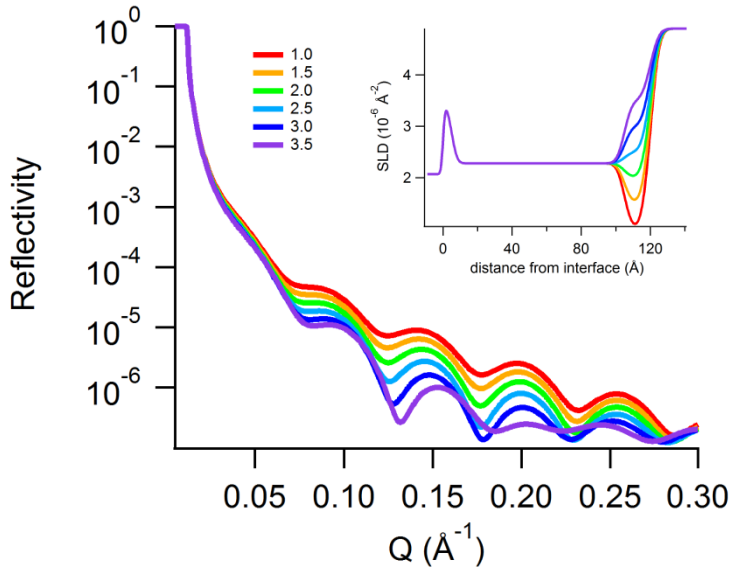


Figure S11 Simulated reflectivity and (inset) SLD profiles for a 15 Å thick dye-layer of varying SLD. Roughness has been fixed at 4 Å, along with all other parameters at the calculated values highlighted in **Table 2** of the main manuscript.

As described in the manuscript, it was necessary to fix, limit, or link a number of structural parameters in the co-refinement to ensure that the changes observed in reflectivity profiles were solely from the dye layer. As such, the silicon super-phase was fixed with an SLD of 2.07 × 10^{-6} $Å^{-2}$ and interfacial roughness of 1 Å. The native oxide layer was fixed at 5 Å thick with an interfacial roughness of 2.5 Å. TiO_2 SLD was fixed at 2.1 × 10^{-6} $Å^{-2}$ after initial fitting, along with a interfacial roughness of 3.5 Å based on previous XRR studies. TiO_2 thickness was linked and co-refined across all three runs on a sample. The surface roughness of the dye-layer was also fixed at values based upon the initial XRR study due to the equivocal nature of the fitted model to this parameter.

4 Rationalisation for a change in sub-phase SLD between solutions 1-3

It was observed that the SLD of the solution 1 solvent sub-phase fell under the calculated value of 4.92 × 10^{-6} $Å^{-2}$ to 4.60 × 10^{-6} $Å^{-2}$ and 4.51 × 10^{-6} $Å^{-2}$ for **MK-2** and **MK-44**, respectively.

This lower than expected SLD for solution 1 can be attributed to a lower than expected d_3-MeCN purity – the literature values for the mass density of d_3-MeCN and h_3-MeCN are 0.844 g cm^{-3} and 0.786 g cm^{-3}, respectively. The mass density of a freshly-opened vial of d_3-MeCN was measured using an Anton-Paar DMA 5000 density meter and was observed to actually be 0.839 g cm^{-3}. Comparing the literature mass density values of the MeCN isotopologues indicates that the actual sample must have a deuterated purity of ~92% in order to obtain the measured mass density (the remaining 8% being the hydrogenated form). Calculating the SLD for this d_3/h_3-MeCN mixture (**Equation 2**) yields an SLD of 4.58×10^{-6} $Å^{-2}$, in close agreement with the value observed with NR.

Upon addition of LiI to the MeCN solvent, to form solution 2, the observed SLD is seen by NR to increase to 4.74×10^{-6} $Å^{-2}$ and 4.67×10^{-6} $Å^{-2}$ for **MK-2** and **MK-44**, respectively. Interestingly, a large increase in mass density is also observed to 0.925 g cm^{-3}. The SLD of the neat solvent at this density would be 5.08×10^{-6} $Å^{-2}$ (**Equation 2**), which is higher than observed. The scattering from the Li^+ and I^- ions (with scattering lengths of -2.22 fm and 5.28 fm, respectively)[3] must therefore be non-negligible. The approximate composition of solution 2 was calculated as being 88.8% d_3-MeCN, 7.7% h_3-MeCN and 3.5% LiI. Calculation of the SLD for this mixture at the observed density yields 4.68×10^{-6} $Å^{-2}$ (**Equation 2**), close to the NR-observed value and also notably larger than that observed for solution 1.

Solution 3 sees a further increase in the SLD of the sub-phase to 4.86×10^{-6} $Å^{-2}$ and 4.74×10^{-6} $Å^{-2}$ with the addition of I_2. The density of solution 3 was found to be essentially unchanged relative to solution 2, at 0.924 g cm^{-3}. The low concentration of I_2, 0.05 M would see it only constitute ~0.3 % of the overall solution, but upon calculation led to a small decrease in overall SLD to 4.54×10^{-6} $Å^{-2}$ (**Equation 2**). This is contrary to that observed with NR. However, the density of solution 3 was found to increase gradually over time (*e.g.* the mass density of

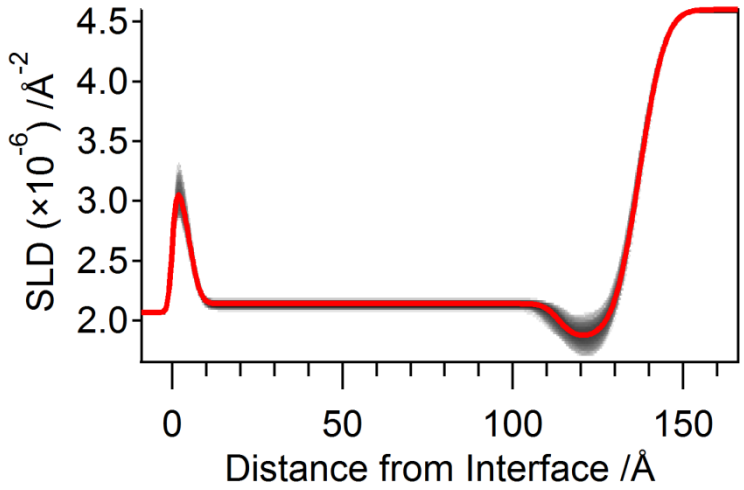
solution 3 after a period of months had exceeded 1.10 g cm^{-3}), possibly due to the hydrophobic nature of the d_3/h_3-MeCN:LiI:I_2 mixture, or gradual evaporation of more volatile components. Due to the time between successive NR measurements, it is possible these effects led to the density of solution 3 increasing to an extent that the decrease in SLD from the addition of I_2 was overcome. Incidentally, a density of 0.985 g cm^{-3} would be required for to obtain an SLD of 4.86×10^{-6} $Å^{-2}$.

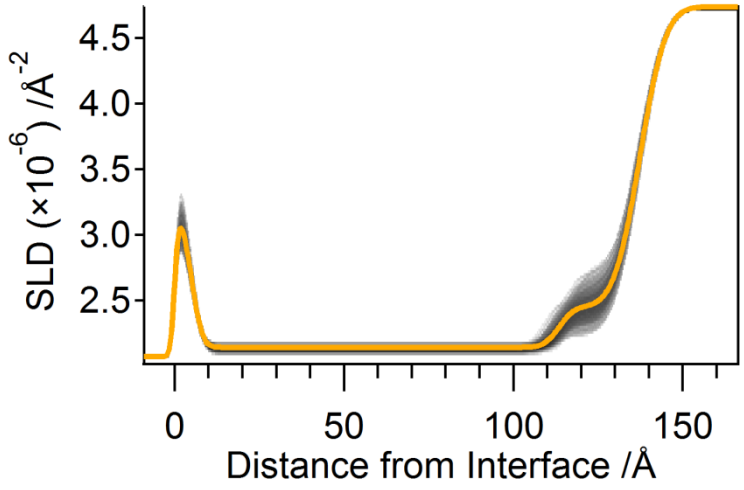
5 Monte-Carlo Resampling of NR data

Monte-Carlo analysis is undertaken after the best fits have been achieved through 'standard' fitting of the NR datasets to a physical model. The fits presented in Figure 5 and the parameters in Table 3 of this paper are a result of fitting with Motofit, but the errors come from the Monte Carlo process. No two fits to data give exactly the same numerical outputs, so Monte-Carlo analysis is then undertaken to give an indication of the spread of fits that satisfy the data. The SLD profiles corresponding to the fits from all the iterations performed are then shown in **Figure S12** (MK-2) and **Figure S13** (MK-44), where the solid line is the Motofit output. It can be seen that the spread of profiles is much tighter for the MK-2 dye, thicker layer with better contrast, than for the MK-44. One can see from these profiles that the fit for the MK-44 solution 1 (**Figure S13a**) is less well determined; this is for a situation where the dye thickness is at the lower limit of detection and there is only a single contrast available for fitting. For **Figure S12b** and **Figure S12c** there is reduced spread of SLD values; note the thickness is very well determined in each case. The errors presented in Table 3 of the paper are a result of the analysis of the spread of values for each parameter around the best fit value.

In more technical detail, resampling of the NR data was conducted to allow calculation of errors in the fitted models using 1000 Monte-Carlo iterations.[4] In these instances, these errors

are presented as one standard deviation (1σ). After each resampling run, an SLD profile indicating the spread of the calculated data are generated and are shown in **Figure S12** for **MK-2** and **Figure S13** for **MK-44**, respectively. It should be noted that **Figures S12** and **S13** show all outcomes of the Monte-Carlo analysis, whereas the values reported in **Table 3** of the manuscript show the median of these values with an error equal to 1 standard deviation.


SLD (×10^{-6}) /Å^{-2}
4.5
4.0
3.5
3.0
2.5
2.0
0
50
100
150
Distance from Interface /Å


SLD (×10^{-6}) /Å^{-2}
4.5
4.0
3.5
3.0
2.5
0
50
100
150
Distance from Interface /Å

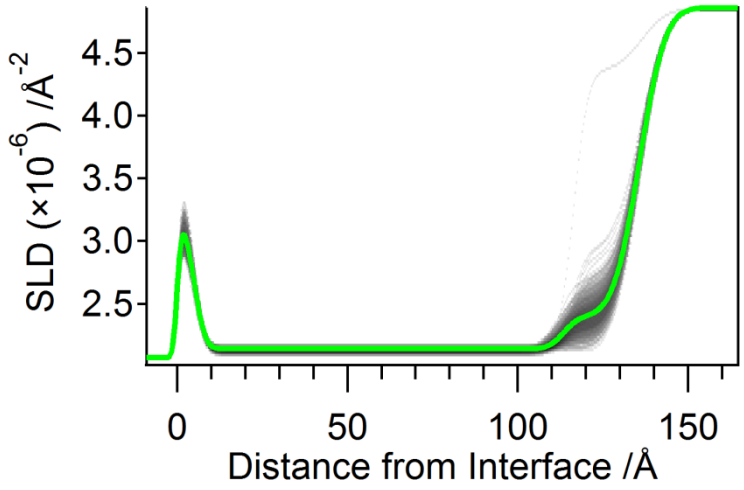
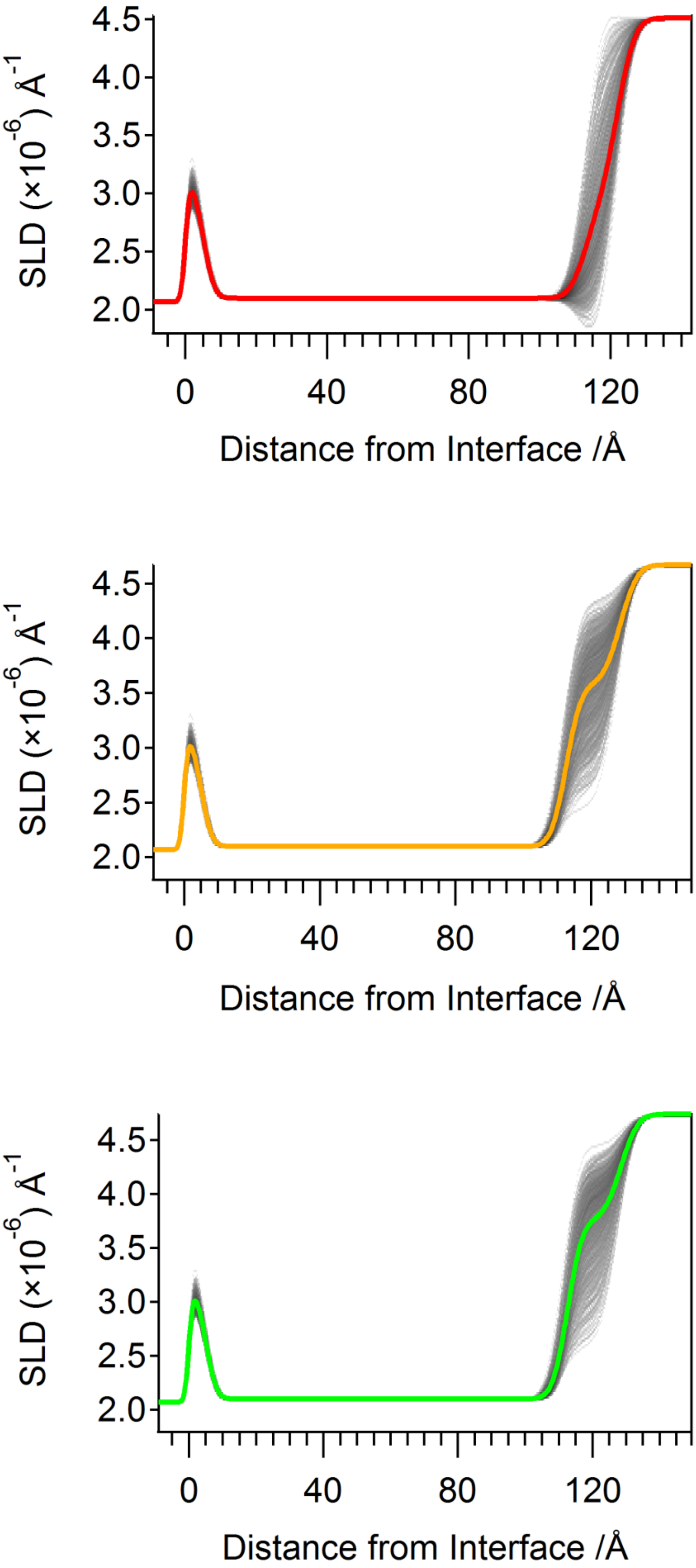

SLD (×10^{-6}) /Å^{-2}
4.5
4.0
3.5
3.0
2.5
0
50
100
150
Distance from Interface /Å

Figure S12 Monte-Carlo resampled SLD profiles for **MK-2**-sensitised TiO_2 surfaces in solutions 1 (top); 2 (middle); and 3 (bottom). The breadth of distribution is indicated by the grey shadowing, where darker regions represent high density. In the **MK-2** example, clear higher density states exist at SLDs of 1.9×10^{-6} Å^{-2} (top) and ~2.4×10^{-6} Å^{-2} (middle and bottom), indicated by the darker colouration, with a spread of approximately 0.1×10^{-6} Å^{-2}.



SLD (×10^{-6}) Å^{-1}
4.5
4.0
3.5
3.0
2.5
2.0
0
40
80
120
Distance from Interface /Å
SLD (×10^{-6}) Å^{-1}
4.5
4.0
3.5
3.0
2.5
2.0
0
40
80
120
Distance from Interface /Å
SLD (×10^{-6}) Å^{-1}
4.5
4.0
3.5
3.0
2.5
2.0
0
40
80
120
Distance from Interface /Å

Figure S13 Monte-Carlo resampled SLD profiles for **MK-44** sensitised TiO_2 surfaces in solutions 1 (top); 2 (middle); and 3 (bottom). Although a higher density region in SLD calculation is not as apparent compared with the **MK-2** example (hence the higher reported error in manuscript Table 3), the change in dye-layer thickness is clearly evident when comparing solution 1 (top) to solutions 2 and 3 (middle and bottom, respectively).

6 Measuring Dye···Li^+ Interaction Using UV-Vis Absorption Spectroscopy

UV-Vis absorption spectroscopy has been successfully demonstrated as a tool for measuring dye···Li^+ interactions, whereby a red shift in the absorption spectrum of the dye species is attributable to complexation of Li^+ cations with carbonyl oxygen atoms.[6] To this end, UV-vis absorption spectroscopy has been employed to confirm the presence of such dye···Li^+ interactions in the case of **MK-44**.

Figure S14 shows a distinct red-shift in **MK-44** absorption after treatment with the lithium iodide, of 21 nm. This is in good agreement with the presented computational results, which indicate that in the presence of Li^+ cations, **MK-44** surface geometry shifts to prefer a lower energy bidentate bridging configuration, which would thus stabilise the dye's electronic structure. A slight decrease in absorption intensity after LiI treatment is suggestive of some dye-desorption, and would corroborate the decrease in **MK-44** surface coverage between solutions 1 and 2.

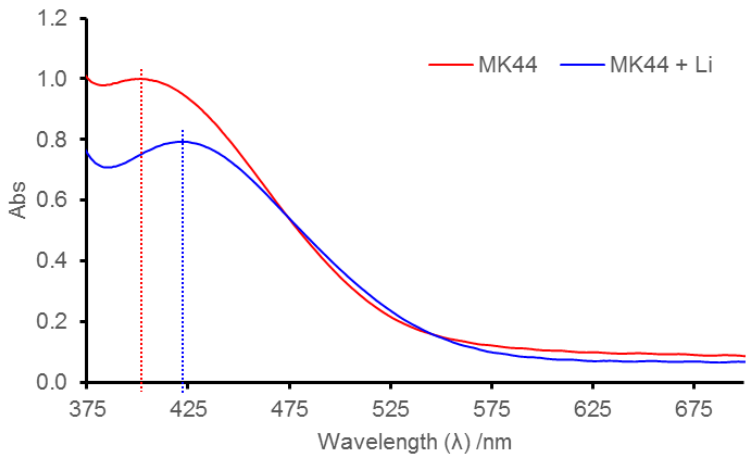


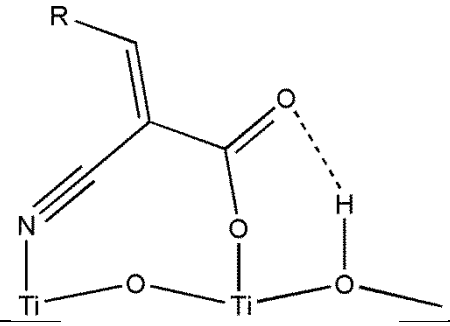
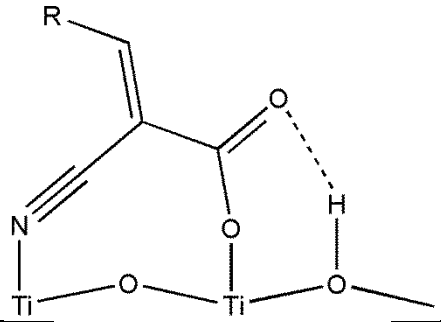
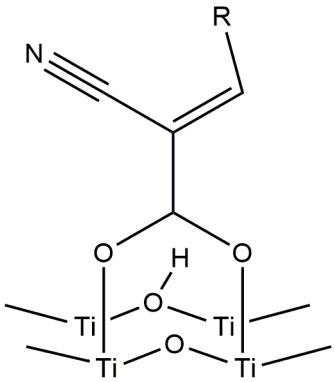
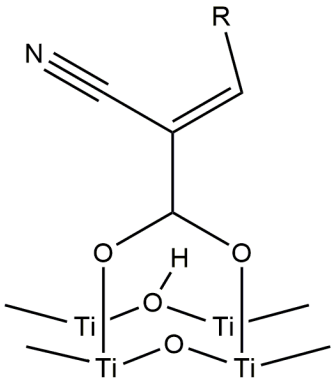
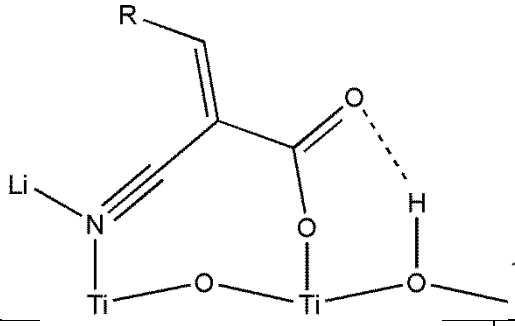
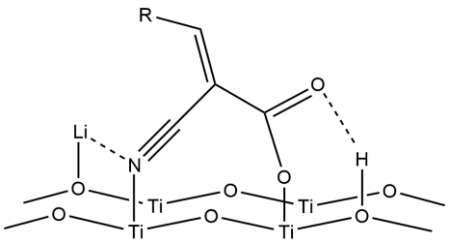
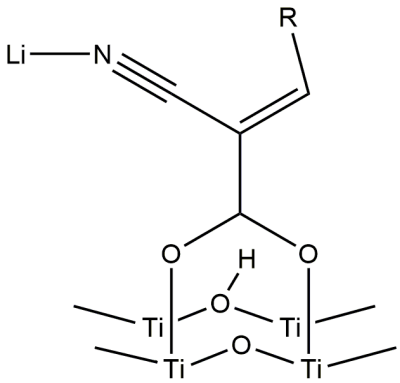
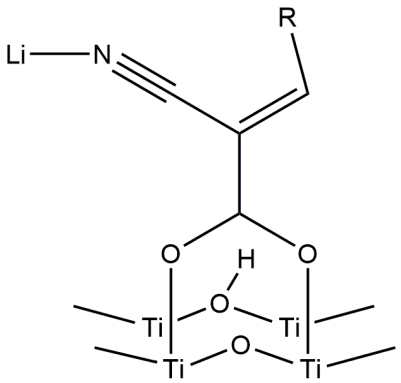
Figure S14 UV-Vis absorption spectra for an **MK-44** sensitised TiO_2 film prior to (red trace) and post (blue trace) lithium iodide treatment. A distinct red-shift of 21 nm is observable after lithium iodide treatment. Absorption intensity has been normalised to the pre-treatment film.

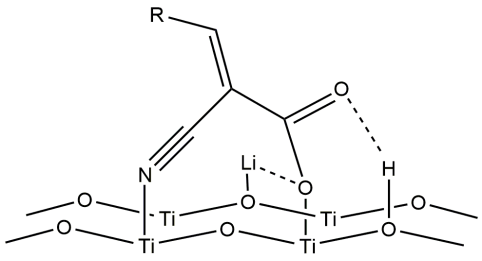
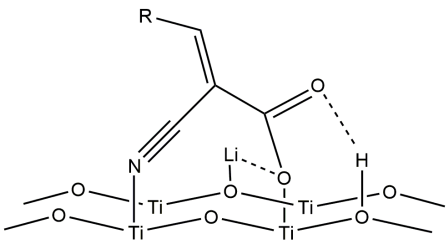
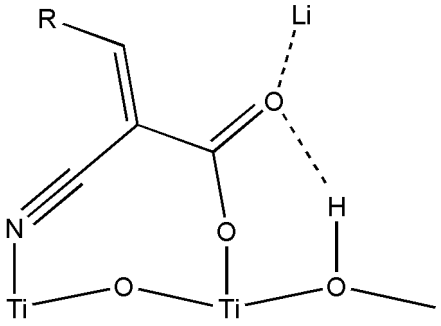
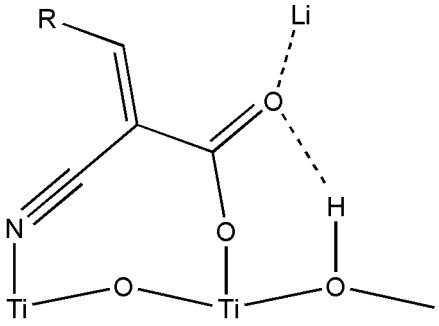
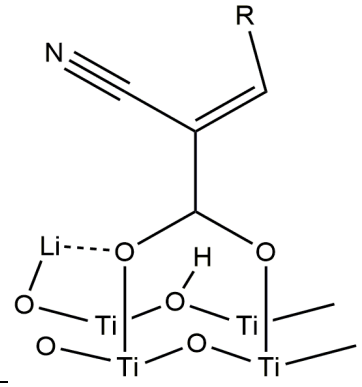
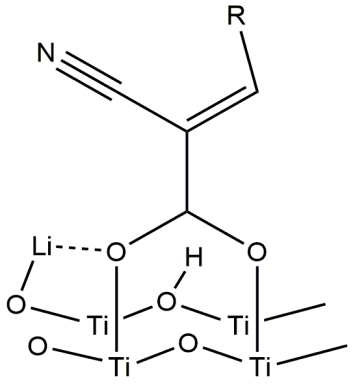
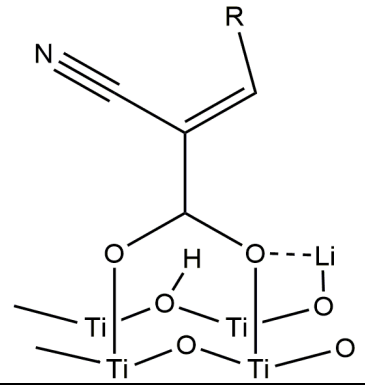
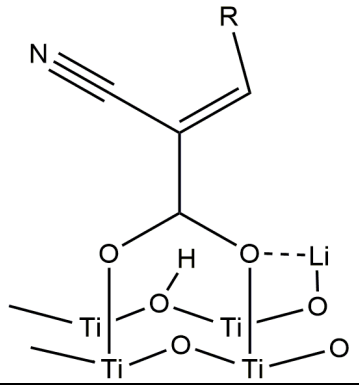
7 Computational Modelling of MK-44 Adsorption

Computational models were constructed to measure the energy difference between the bidentate bridging and CN/COO binding modes to a TiO_2 surface in the absence and presence of lithium cations.

The final energy of the computational models are shown in **Table S3**, where the most stable structures are represented by the most negative changes in adsorption energy, ΔE^a between the various DFT models of **MK-44** on TiO_2 in the absence and presence of Li^+ ions (CN/COO and BB_Li_O_1, respectively).

Table S3 Final energies of computational **MK-44** molecules. * denotes the most stable structures in the absence and presence of Li^+ ions.

DFT modelling of the MK-44 dye on a TiO_2 surface where no Li+ ions exist				
Adsorption Mode	Starting Structure	Final Structure	Adsorption Energy (eV)	ΔE^a (eV)
CN/COO (no Li^+ ions are present)			-7.60	0*
BB (no Li^+ ions are present)			-7.41	0.19
DFT modelling of the MK-44 dye on a TiO_2 surface where Li^+ ions are present				
Adsorption Mode	Starting Structure	Final Structure	Energy (Hartree)	ΔE^b (eV)
CN/COO _Li_N			-10514.31131	0
BB_Li_N			-10514.28229	0.79

CN/COO _Li_O_1			-10514.31178	-0.01
CN/COO _Li_O_2			-10514.28441	0.73
BB_Li_O_1			-10514.31558	-0.12*
BB_Li_O_2			-10514.28777	0.64

Optimized atomic coordinates for each model are given below.

MK44_CN/COO **atomic coordinates**

O	-0.61476700	0.82465800	-0.97005600
O	-1.53800400	-1.86832200	-2.21968400
Ti	-1.04766500	2.48995900	-0.07250800
Ti	-1.92534900	-0.28643700	-1.25951900

O	-1.84398500	3.21602500	-1.38269800
Ti	-2.72050800	-3.14429400	-1.77871000
O	-3.38661900	0.76081900	-1.84768100
O	-1.51895900	3.65485600	1.34499700
O	-4.29113700	-3.76633300	-2.52115700
O	-2.67839000	-3.53494400	-0.02985100
O	-2.27879300	-0.89935900	0.44353900
O	-3.88361900	-1.73756000	-1.25165200
Ti	-3.85208100	2.82864400	-1.53688900
O	-2.68161400	1.65805700	0.54560600
O	-4.26210800	3.62718200	-2.88829900
Ti	-5.04347600	0.16840400	-1.11106500
Ti	-5.49991800	-2.72388400	-1.55780900
O	-5.53662300	1.79606900	-1.07995500
Ti	-3.25252500	3.20589400	1.51351900
Ti	-3.76242100	-2.18333000	0.73521000
O	-6.21224100	-1.12502900	-1.88662800
Ti	-3.29750900	0.35831300	1.85324200
O	-4.10736300	3.83985700	0.16066200
O	-4.67414700	-0.34196600	0.68509300
O	-5.39026300	-3.03750100	0.19448100
O	-3.95582100	1.82047700	2.63081100
O	-3.51656700	-1.61989600	2.52653300
O	-1.61740800	0.31084100	2.78452400
C	-0.73920400	-0.67926600	2.92765200
O	-1.06962500	-1.81673800	3.35792800
C	0.64461900	-0.35089700	2.51080000
C	1.63542000	-1.28125500	2.70588000
C	0.77556900	0.86297400	1.81012900
H	1.29850800	-2.17728000	3.22374200
C	2.99666700	-1.25672800	2.34256000
N	0.76689100	1.85398500	1.18751100
S	3.78720600	0.02260600	1.43090200
C	3.91823300	-2.26686500	2.64519100
C	5.32400000	-0.79935600	1.48881400
C	5.21136300	-2.01205500	2.17447100
H	3.63965500	-3.14904100	3.20593000
C	6.51344400	-0.23395400	0.86861700
H	6.05037400	-2.66935000	2.34609100
C	7.62736600	-1.05288000	0.59286300
C	6.56836000	1.14294700	0.52374900
H	7.59563300	-2.11069600	0.82273700
C	8.75318800	-0.50644000	-0.00663900
C	7.68219800	1.70562000	-0.07858400
H	5.72177100	1.78012200	0.75324100
C	10.03059700	-1.06339600	-0.42321800
C	8.78229000	0.88304300	-0.34680300
H	7.69139200	2.75858300	-0.32860400
C	10.58947600	-2.34205400	-0.35958600
C	10.77517900	0.00830600	-0.99272800
N	10.00404800	1.17937400	-0.92864700
C	11.87374800	-2.54210600	-0.86248200
H	10.03337300	-3.16583200	0.07272700
C	12.06010200	-0.19225600	-1.49827800
C	10.39778100	2.48745400	-1.48040900

H	12.32092900	-3.52773800	-0.82236800
C	12.59808000	-1.47664100	-1.42492100
H	12.62747200	0.61815400	-1.93801900
H	11.47784700	2.59527000	-1.34382200
H	9.91133300	3.26328300	-0.88203100
C	10.01799000	2.62647500	-2.96843200
H	13.59443200	-1.65559700	-1.81136000
H	10.32779400	3.60697800	-3.34491400
H	8.93609800	2.52570300	-3.09519700
H	10.51047300	1.84947500	-3.56041300
H	-2.65137300	-1.88270200	3.05141400

MK44_BB atomic coordinates

O	-0.55909600	-0.49352700	-0.80668600
O	-0.64700100	-1.82363100	1.03671500
O	-2.77693400	-0.97549500	2.35458100
O	-3.54403600	2.07030300	2.89539900
Ti	-2.67010500	-2.46643300	1.11522300
Ti	-3.61034100	0.49400400	1.89592400
O	-4.26532400	-3.15096300	1.20850900
Ti	-3.91183900	3.46663500	1.78202300
O	-5.20660500	-0.15633600	1.38078200
O	-2.01811100	-3.60782500	-0.29978500
O	-5.52379000	4.24291900	1.32687900
O	-2.70233200	3.73146700	0.50504100
O	-2.33167100	1.04280000	0.46002000
O	-4.56080100	2.14391800	0.59863000
Ti	-5.60303400	-3.06774100	-0.21475000
O	-3.15888800	-1.44030000	-0.38600600
O	-6.79484000	-4.14907200	0.00442600
Ti	-5.68776700	0.21458400	-0.34838100
Ti	-5.92527000	3.22705600	-0.18011900
O	-6.27386100	-1.34564400	-0.80210100
Ti	-2.86866900	-2.84330500	-1.66152600
Ti	-3.24238600	2.48908500	-0.89623000
O	-6.83759000	1.71707000	-0.45828200
Ti	-2.31309900	-0.04089000	-1.52617700
O	-4.47732400	-3.49822300	-1.71119500
O	-4.11920900	0.70646000	-1.31177400
O	-4.72704600	3.50642900	-1.47778300
O	-2.34451500	-1.34946600	-2.73236200
O	-2.00529000	1.78553500	-1.97809000
C	0.02306400	-1.16837800	0.17672100
C	1.48135300	-1.11448000	0.25442400
C	2.18798100	-0.39800900	-0.68045000
C	2.07325600	-1.83647500	1.31853800
H	1.58149400	0.09103400	-1.43851900
C	3.58147000	-0.20323300	-0.80577700
N	2.54857100	-2.43609400	2.20041600
S	4.81401600	-0.84037900	0.27569200
C	4.18050800	0.54308200	-1.82712700
C	6.09370600	-0.11722900	-0.66108200
C	5.57837500	0.58997200	-1.74870600
H	3.59987300	1.02017300	-2.60576000
C	7.49459700	-0.27736100	-0.28879400

H	6.20194800	1.09261000	-2.47277800
C	8.46705200	0.61153700	-0.78775100
C	7.89924000	-1.32431600	0.58086600
H	8.17423100	1.43357800	-1.42923500
C	9.79851500	0.45005500	-0.42818900
C	9.22302500	-1.49870100	0.95438800
H	7.15587800	-2.02170200	0.94993800
C	11.01474500	1.17789500	-0.75419300
C	10.18042600	-0.61281800	0.44875900
H	9.49880700	-2.30757100	1.61858500
C	11.28432200	2.29290400	-1.55141600
C	12.07721600	0.52405700	-0.06705600
N	11.55219300	-0.56185900	0.64872700
C	12.59822800	2.74591300	-1.65578900
H	10.48437100	2.79867400	-2.07976000
C	13.39250100	0.97913600	-0.16980000
C	12.32330100	-1.44775300	1.53667300
H	12.82362900	3.60987200	-2.26891000
C	13.63835100	2.09345700	-0.97119400
H	14.20270600	0.48907100	0.35524800
H	13.31818300	-1.57546400	1.09965600
H	11.83602200	-2.42719400	1.53758000
C	12.42444700	-0.88767100	2.97002800
H	14.65233000	2.46378900	-1.06551900
H	13.00521000	-1.56956700	3.60010000
H	11.42658800	-0.77057800	3.40289800
H	12.91563700	0.08980700	2.96167000
H	-1.39125800	1.22842800	0.71420900

MK44_CN/COO _Li_N atomic coordinates

O	-0.52952600	0.80115100	-0.81034100
O	-1.44108000	-1.91534300	-2.10700300
Ti	-1.04482400	2.41954500	-0.03057900
Ti	-1.84765500	-0.33799300	-1.19708500
O	-1.76834400	3.20097900	-1.33654500
Ti	-2.65136000	-3.19869500	-1.71455300
O	-3.27049500	0.72066300	-1.82918400
O	-1.51793700	3.66030600	1.47292000
O	-4.19316600	-3.81332600	-2.49805700
O	-2.68274900	-3.54753900	0.04264400
O	-2.29196800	-0.89032600	0.48154200
O	-3.82962300	-1.77350300	-1.24995200
Ti	-3.79158900	2.79931600	-1.58373900
O	-2.68681700	1.67353400	0.57330900
O	-4.12169100	3.58282700	-2.95821100
Ti	-4.97620000	0.13492600	-1.17777700
Ti	-5.45001600	-2.76103900	-1.61501100
O	-5.45848400	1.76936100	-1.19579500
Ti	-3.31067600	3.21326000	1.51047600
Ti	-3.80517900	-2.20282400	0.73862700
O	-6.11435700	-1.15270600	-1.98317700
Ti	-3.35290800	0.35051700	1.85909900
O	-4.09833100	3.82623900	0.12379700
O	-4.67877200	-0.33707100	0.64083900

O	-5.40028400	-3.03415700	0.15313400
O	-4.03654500	1.84675500	2.58776600
O	-3.57924500	-1.59418400	2.52431600
O	-1.68325900	0.33576100	2.81672200
C	-0.79715200	-0.67028000	2.90604700
O	-1.13045700	-1.82138500	3.28624300
C	0.57843900	-0.32538300	2.49216000
C	1.55970400	-1.32179400	2.53421300
C	0.72869600	0.96187900	2.00903700
H	1.20150800	-2.25374400	2.96790200
C	2.87996500	-1.30875200	2.11315500
N	0.72891800	2.07711800	1.60995100
S	3.70172200	0.03821200	1.31873100
C	3.77597800	-2.39741200	2.24822400
C	5.19200100	-0.86552800	1.18199200
C	5.04100000	-2.15372100	1.74450800
H	3.47303500	-3.33027400	2.70478700
C	6.36688300	-0.31554100	0.56246700
H	5.83592300	-2.88295700	1.75466900
C	7.59983500	-1.01563500	0.62025700
C	6.31927800	0.93575800	-0.12144900
H	7.66824200	-1.96056000	1.14357400
C	8.72330500	-0.48023100	0.02321400
C	7.43132200	1.48402600	-0.72801800
H	5.37653500	1.46716100	-0.18743500
C	10.10343000	-0.92917900	-0.09041400
C	8.64684400	0.78328700	-0.65845000
H	7.35791900	2.42843300	-1.25078300
C	10.78818800	-2.05902900	0.36123600
C	10.79363400	0.06897800	-0.82963600
N	9.88679800	1.10015400	-1.15489400
C	12.14651800	-2.18022900	0.07085600
H	10.27647200	-2.82857100	0.92701300
C	12.15065300	-0.05025300	-1.12266700
C	10.22117600	2.29239600	-1.96184700
H	12.69427600	-3.04950500	0.41240200
C	12.81683700	-1.18640700	-0.66221800
H	12.67856700	0.70581400	-1.68918700
H	11.24119200	2.58929000	-1.70284400
H	9.55335500	3.10149000	-1.65382500
C	10.09503200	2.01906300	-3.47360000
H	13.87211100	-1.30356800	-0.87622400
H	10.36008800	2.91979900	-4.03633600
H	9.06967500	1.73452100	-3.72737700
H	10.76525600	1.20841600	-3.77331900
H	-2.71358400	-1.87452400	3.04570100
Li	-0.01451700	3.76061600	2.36466100

MK44-_BB_Li_N atomic coordinates

O	-0.50620700	-0.18596800	-0.49087800
O	-0.61112300	-1.66358400	1.24976100
O	-2.96773900	-1.04807900	2.33556600
O	-4.08895700	1.87726700	2.98087000

Ti	-2.63960700	-2.42043900	1.02024900
Ti	-3.90588100	0.37737600	1.89577500
O	-4.12983800	-3.30030700	0.91489900
Ti	-4.48969800	3.30653200	1.91339900
O	-5.35734600	-0.39400000	1.17672300
O	-1.68785000	-3.39106000	-0.36576200
O	-6.11624600	3.93310400	1.32625900
O	-3.18663300	3.76001300	0.78541900
O	-2.54584600	1.11497700	0.62881500
O	-4.86449400	1.99941600	0.59779700
Ti	-5.30715900	-3.26759600	-0.65829400
O	-3.06168700	-1.36524900	-0.46025300
O	-6.38764900	-4.47583300	-0.64315000
Ti	-5.69579900	0.01357900	-0.57880700
Ti	-6.26422700	2.98353400	-0.26773100
O	-6.07587800	-1.56418600	-1.16796300
Ti	-2.47205900	-2.64098000	-1.77709900
Ti	-3.45677200	2.57742300	-0.72549500
O	-6.96353300	1.40509100	-0.72078500
Ti	-2.23930400	0.19418000	-1.40046300
O	-3.98118800	-3.45427000	-2.03959800
O	-4.10212900	0.74446600	-1.34508300
O	-4.97048500	3.46518500	-1.40616300
O	-1.98180300	-1.02615500	-2.67113600
O	-2.03717900	2.04894800	-1.69581800
C	0.04564100	-0.93490000	0.43439800
C	1.51683800	-0.91034400	0.52082600
C	2.25196700	-0.10203100	-0.33931600
C	2.03719700	-1.77549000	1.48131400
H	1.62930800	0.47494800	-1.01976500
C	3.62517500	0.08905600	-0.47795500
N	2.41184600	-2.52685400	2.29744200
S	4.89512900	-0.69285800	0.46577300
C	4.20775700	0.96077500	-1.42218100
C	6.15619100	0.13836100	-0.41738800
C	5.59520200	0.98925300	-1.38847400
H	3.60546100	1.53892800	-2.11068600
C	7.55610700	-0.07142700	-0.13866700
H	6.19434100	1.58502800	-2.05933100
C	8.53199400	0.77497200	-0.72014500
C	7.98521000	-1.12646300	0.71673400
H	8.23253900	1.59575300	-1.35904900
C	9.87189200	0.56687400	-0.45263900
C	9.32033400	-1.35142900	0.99421400
H	7.24448600	-1.78974900	1.14896800
C	11.09021200	1.23982900	-0.87731700
C	10.27718000	-0.50731300	0.41005300
H	9.61390600	-2.16583900	1.64338600
C	11.34607100	2.33438800	-1.70624900
C	12.16977800	0.54771500	-0.26411200
N	11.64930400	-0.51184200	0.50646500
C	12.66811200	2.72504300	-1.91233600
H	10.53386500	2.87172700	-2.18148800
C	13.49245100	0.93711300	-0.46818500
C	12.45725100	-1.42893500	1.33514600

H	12.88593200	3.57171500	-2.55114800
C	13.72647300	2.03239700	-1.29969000
H	14.31697700	0.41473000	-0.00054400
H	13.39888500	-1.60664300	0.80831400
H	11.92638500	-2.38337900	1.39166500
C	12.71623100	-0.85871800	2.74368700
H	14.74553400	2.35502800	-1.47481700
H	13.32457800	-1.56075300	3.32292500
H	11.77108200	-0.69381200	3.26948100
H	13.24783500	0.09486700	2.67825800
H	-1.65532600	1.36008000	0.98929900
Li	2.56804400	-3.82532600	3.57486300

MK44_CN/COO_Li_O_1 atomic coordinates

O	-1.46475900	0.77909900	-1.57514400
O	-4.07869200	0.36301600	-3.25814300
Ti	-0.64243500	1.47001900	0.08872000
Ti	-3.25090000	0.69439300	-1.62212000
O	-1.38084100	2.98802900	0.17991100
Ti	-5.51704100	-0.71691000	-3.02172400
O	-4.01634100	1.92343400	-0.45037200
O	0.02607900	1.22314700	1.84561600
O	-7.30884900	-0.43127900	-2.75410700
O	-5.06508000	-2.29418200	-2.30201600
O	-3.17728600	-1.02385300	-0.91561800
O	-5.47718600	-0.12149000	-1.20761800
Ti	-3.18824000	3.06890500	1.17945200
O	-2.15990600	0.61188400	0.95707500
O	-3.55611000	4.64127600	1.14619300
Ti	-5.33850000	1.10654300	0.67449600
Ti	-7.36996200	-0.39460800	-0.89750300
O	-4.86994100	2.18217800	1.89452700
Ti	-1.49021000	0.92309500	2.73398900
Ti	-4.92280700	-1.92057000	-0.45025200
O	-7.19283000	0.93206000	0.25773000
Ti	-2.75217600	-1.20419100	1.25851300
O	-2.30254600	2.42879800	2.84221900
O	-4.60565000	-0.60587800	1.07671800
O	-6.77379000	-1.93953100	-0.18479800
O	-2.24474400	-0.87128300	2.90204300
O	-3.78523800	-2.92460700	0.73514700
O	-1.06959900	-1.82550300	0.43802000
C	-0.01137800	-2.57980800	0.94426300
O	-0.20052100	-3.60758200	1.59159900
C	1.31644700	-2.01453900	0.60672800
C	2.44818800	-2.71126700	1.02773400
C	1.29886600	-0.77849300	-0.03648400
H	2.21447900	-3.64525600	1.53612300
C	3.79688700	-2.39976200	0.90332100
N	1.12526000	0.26841100	-0.54880800
S	4.45187900	-0.94318400	0.15273400
C	4.85579900	-3.20929300	1.37409800
C	6.09555100	-1.43007000	0.48940400
C	6.11592500	-2.67974200	1.14482800

H	4.67538100	-4.15113800	1.87494400
C	7.22343100	-0.61153600	0.12501200
H	7.02975900	-3.15989700	1.45857400
C	8.54137900	-1.12138100	0.23265200
C	7.03865300	0.72088800	-0.34766400
H	8.70944300	-2.13495800	0.57333600
C	9.61647900	-0.32875000	-0.12034700
C	8.10151200	1.52878500	-0.70110900
H	6.03455500	1.12416500	-0.41643400
C	11.05557300	-0.54671800	-0.13238700
C	9.40187800	1.01179400	-0.59003400
H	7.92621100	2.53760800	-1.05059300
C	11.86809200	-1.63033900	0.20755900
C	11.64354100	0.66026100	-0.59916400
N	10.61816300	1.59149800	-0.86281000
C	13.24998300	-1.49960500	0.07743100
H	11.43514500	-2.55687000	0.56588400
C	13.02460400	0.79314800	-0.73074300
C	10.82987600	2.94584000	-1.41345700
H	13.89568900	-2.32966500	0.33535500
C	13.81852300	-0.30092700	-0.38588300
H	13.47518600	1.70944500	-1.08966000
H	11.76000500	3.33256700	-0.98776500
H	10.01483600	3.58222200	-1.05793100
C	10.89204500	2.93976000	-2.95354000
H	14.89491200	-0.22349600	-0.47892400
H	11.06076800	3.95669500	-3.32199000
H	9.95398100	2.56441800	-3.37301600
H	11.70892300	2.30055300	-3.30049000
H	-3.47005800	-3.85752600	0.82018800
Li	-1.35458600	-1.17849100	-1.29791900

MK44_CN/COO_Li_O_2 atomic coordinates

O	-0.55826800	0.93695400	-0.86705800
O	-1.46743500	-1.59167700	-2.40850500
Ti	-0.99241400	2.50674100	0.19300700
Ti	-1.86807700	-0.12852700	-1.28157300
O	-1.79191800	3.35367400	-1.03630300
Ti	-2.65268100	-2.90889500	-2.16065000
O	-3.32027700	0.98086300	-1.76836400
O	-1.48554300	3.50099600	1.72491200
O	-4.20937600	-3.41609600	-2.99883200
O	-2.65525900	-3.49734400	-0.45479200
O	-2.24526200	-0.94361000	0.34239100
O	-3.82646000	-1.56665900	-1.48434300
Ti	-3.79080900	3.01138400	-1.27327200
O	-2.61177100	1.58407200	0.72908000
O	-4.17809900	3.95774500	-2.52670800
Ti	-4.99717300	0.32672300	-1.15358300
Ti	-5.44813700	-2.50083800	-1.95411000
O	-5.48600500	1.93751600	-0.95202000
Ti	-3.21859900	3.03652500	1.83599600
Ti	-3.75663500	-2.24441800	0.40989500
O	-6.13604900	-0.87309000	-2.10223800

Ti	-3.29664800	0.16337300	1.82572400
O	-4.05197300	3.79297400	0.54466300
O	-4.64726300	-0.38994900	0.58927000
O	-5.36634200	-3.00904000	-0.23489300
O	-3.95162000	1.51563900	2.76760700
O	-3.54837700	-1.89370300	2.29633200
O	-1.64875000	-0.03724100	2.89701200
C	-0.72119800	-0.93793700	3.04866200
O	-1.02008500	-2.08821000	3.60199200
C	0.61407500	-0.63090700	2.58684800
C	1.63601500	-1.58095200	2.64971800
C	0.73933200	0.62867500	1.96811800
H	1.34296000	-2.52645100	3.09820600
C	2.95251700	-1.51049700	2.21218800
N	0.74738200	1.66966800	1.43581400
S	3.71006200	-0.12339800	1.42409300
C	3.89585000	-2.56120500	2.32944900
C	5.23841400	-0.95436000	1.28095500
C	5.14598000	-2.25846000	1.82171000
H	3.64117500	-3.51033200	2.78236400
C	6.38845000	-0.33465300	0.68046500
H	5.97773700	-2.94525500	1.83876800
C	7.59731700	-1.06064900	0.52493200
C	6.33731400	1.01790500	0.22747200
H	7.66403400	-2.08988000	0.85298300
C	8.69361900	-0.45505400	-0.05569700
C	7.42298300	1.63938800	-0.35471900
H	5.41902900	1.58233600	0.34411400
C	10.04367100	-0.91023600	-0.35558400
C	8.61406000	0.90935100	-0.50115900
H	7.34857600	2.66557000	-0.68904900
C	10.71733200	-2.11794600	-0.16364700
C	10.71481800	0.18640800	-0.96107600
N	9.82544800	1.27956500	-1.03036900
C	12.04522700	-2.21824300	-0.57698800
H	10.21992500	-2.96304100	0.29747900
C	12.04147300	0.08880700	-1.37569000
C	10.14072700	2.58603700	-1.64579200
H	12.58356800	-3.14727200	-0.43726200
C	12.69687400	-1.12647900	-1.17502400
H	12.55409800	0.92096100	-1.84047700
H	11.18902800	2.80782000	-1.42768300
H	9.53185000	3.34500500	-1.14715400
C	9.88354400	2.58431400	-3.16553800
H	13.72862200	-1.22885800	-1.48834100
H	10.13731400	3.56303200	-3.58493800
H	8.83084700	2.37375300	-3.37560600
H	10.49588800	1.82260100	-3.65648900
H	-2.72714000	-2.21129800	2.78405300
Li	-1.40794200	-2.94161000	5.01420800

MK44_BB_Li_O_1 atomic coordinates

O	-1.23487800	-1.97468700	-1.33825900
O	-1.34913400	-2.73383400	0.81559900

O	-2.46354300	-1.09741000	2.32889600
O	-1.51481800	1.92839100	2.49917600
Ti	-3.55506200	-2.39872200	1.18810700
Ti	-2.56798400	0.61126500	1.76787500
O	-5.19673300	-2.15051600	1.66898000
Ti	-1.38426800	3.32203800	1.29151000
O	-4.32861600	0.83223700	1.63267300
O	-3.79242700	-3.75756600	-0.07138500
O	-2.45007600	4.78803100	1.02883100
O	-0.53899300	2.87521200	-0.20451500
O	-1.55752900	0.36094100	0.05541600
O	-2.85239200	2.48106400	0.44583100
Ti	-6.59105100	-1.49104200	0.44549000
O	-3.71694900	-1.32857400	-0.31921500
O	-8.09062300	-1.80830200	0.96159400
Ti	-4.97527400	1.37185200	-0.01092600
Ti	-3.65323500	4.10086600	-0.21782900
O	-6.34493000	0.33212200	-0.14058400
Ti	-4.40662800	-2.74586700	-1.44554100
Ti	-1.92806300	2.07146000	-1.30526600
O	-5.21151400	3.23689300	-0.10669200
Ti	-2.57050400	-0.58347200	-1.77610000
O	-6.08026800	-2.47687300	-1.14059400
O	-3.63312100	0.98115600	-1.30631800
O	-2.80181000	3.67970500	-1.73221300
O	-3.52685900	-1.70111300	-2.76942700
O	-1.47323600	0.79050700	-2.47752000
C	-0.66248900	-2.30483800	-0.20502900
C	0.76122500	-2.05372500	-0.03853300
C	1.55990800	-1.67049100	-1.11989300
C	1.14800100	-2.14546100	1.31421600
H	1.03073600	-1.60195900	-2.06798500
C	2.91388800	-1.37273000	-1.15627800
N	1.21327400	-2.18993900	2.48599800
S	4.02087100	-1.44202500	0.21763500
C	3.61994100	-0.97282300	-2.31820600
C	5.37823900	-0.95329200	-0.76942100
C	4.96644900	-0.73986500	-2.10608000
H	3.12886000	-0.87247900	-3.27729800
C	6.70265600	-0.81586400	-0.22961800
H	5.64923500	-0.44478500	-2.88743200
C	7.75107500	-0.28650000	-1.02646300
C	6.99107900	-1.20915400	1.11179600
H	7.55890300	0.03053900	-2.04331500
C	9.01979400	-0.16055300	-0.49772600
C	8.25382900	-1.09317000	1.65574100
H	6.19914800	-1.62614600	1.72364900
C	10.28029900	0.33391900	-1.03305000
C	9.28263800	-0.56850400	0.85573400
H	8.43914400	-1.40404000	2.67532300
C	10.66213400	0.85582100	-2.27044800
C	11.24021900	0.20244900	0.00644500
N	10.60826100	-0.35463000	1.13880300
C	11.98978500	1.23993500	-2.45528600
H	9.94291100	0.96111800	-3.07407000

C	12.56713900	0.58657200	-0.17489600
C	11.26870100	-0.59830900	2.43853700
H	12.30435300	1.64695000	-3.40804100
C	12.92859400	1.10567100	-1.41858900
H	13.29969200	0.49127000	0.61604700
H	12.29650400	-0.90866400	2.23168500
H	10.76025600	-1.43870200	2.91892000
C	11.24264000	0.65097700	3.34091100
H	13.95402500	1.41150400	-1.58609600
H	11.74962600	0.43512500	4.28672900
H	10.21155100	0.94800000	3.55416500
H	11.75188900	1.48655400	2.85240300
H	-0.58303800	0.16108700	0.09379400
Li	-0.93327200	-2.10492200	2.61645000

MK44_BB_Li_O_2 atomic coordinates

O	-0.61213700	1.28926400	0.50311500
O	-0.67699700	-0.53389700	1.86391400
O	-3.15418500	-1.58127500	2.27472600
O	-5.65553000	0.12506300	2.70190800
Ti	-1.69684900	-2.22709100	1.05901600
Ti	-4.43459900	-0.69621000	1.55903500
O	-2.74575500	-3.38798300	0.38568300
Ti	-6.26479600	1.66430200	1.97767200
O	-4.93690900	-1.59314300	0.00628600
O	-0.26760700	-2.39914700	-0.16171600
O	-7.75934200	2.01654100	0.97202400
O	-5.00249600	2.89733400	1.65301900
O	-3.31244200	0.87185500	1.12763400
O	-5.68032500	0.94213500	0.30754100
Ti	-3.87233900	-3.02352000	-1.23116300
O	-2.24448300	-0.98663700	-0.33151900
O	-4.67527000	-4.39622400	-1.51531000
Ti	-5.28785200	-0.43994900	-1.46563000
Ti	-7.06399400	1.83401200	-0.73234500
O	-4.70888800	-1.65538800	-2.49206100
Ti	-1.01578900	-1.69931900	-1.64036000
Ti	-4.30337400	2.39858500	-0.04960100
O	-6.94344100	0.42690200	-1.80619100
Ti	-2.10595700	0.83252300	-0.85081000
O	-2.16292800	-2.80654100	-2.24941000
O	-3.91565800	0.88541600	-1.38365800
O	-5.75589200	3.03226800	-1.04237200
O	-1.05971200	0.18949300	-2.12106200
O	-2.56074000	2.76506800	-0.44032300
C	0.04007200	0.30912900	1.20950600
C	1.45991800	0.23652200	1.16342600
C	2.21002100	1.07511200	0.33260500
C	2.02908000	-0.81474500	1.92696300
H	1.63474400	1.78978900	-0.25008600
C	3.58183100	1.10002200	0.10727000
N	2.45625200	-1.70258400	2.55257100
S	4.78219000	0.05304100	0.87181100
C	4.22625700	1.97848800	-0.79990000

C	6.08683700	0.79401800	-0.01797300
C	5.59722600	1.81329200	-0.86849300
H	3.67368500	2.70235300	-1.38502200
C	7.45253500	0.36761600	0.13672700
H	6.23561700	2.39540100	-1.51454700
C	8.49459300	1.02234800	-0.56822400
C	7.78474400	-0.72134600	0.99729800
H	8.27362300	1.85388600	-1.22484100
C	9.80054200	0.60101000	-0.41374900
C	9.08401800	-1.15613400	1.16362900
H	6.99498100	-1.23155800	1.53695600
C	11.06677200	1.04491100	-0.97886700
C	10.10548600	-0.50055900	0.45711300
H	9.30126300	-1.98420100	1.82531100
C	11.41906400	2.05307300	-1.87827000
C	12.07134500	0.20101400	-0.43225300
N	11.45916500	-0.73223400	0.42990900
C	12.76207400	2.20893700	-2.21921300
H	10.66476600	2.70378800	-2.30474200
C	13.41437100	0.35560900	-0.77006800
C	12.18134500	-1.74944300	1.22177000
H	13.05416700	2.98591700	-2.91450700
C	13.74551000	1.36884300	-1.67019000
H	14.18232800	-0.28254200	-0.35257000
H	13.02009800	-2.10348600	0.61601000
H	11.50486700	-2.59463000	1.37503800
C	12.67502300	-1.18752000	2.56951500
H	14.78248300	1.50982700	-1.94951600
H	13.21143500	-1.96593200	3.12143700
H	11.82996200	-0.84606000	3.17449700
H	13.35075600	-0.34287600	2.40752900
H	-2.60111800	1.03756700	1.80084900
Li	-1.04022000	3.06817400	0.47146300

8 References

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