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[12] Crystal structure analysis: STOE-IPDS ($\mathrm{Mo}_{\mathrm{K}\alpha}$ radiation); Data collection and refinement (SHELXS-86, SHELXL-93); empirical corrections (habit). **1**: triclinic, space group $P\bar{1}$ (no. 2), $Z=1$, lattice constants (190 K): $a=1770.4(4)$, $b=1849.1(4)$, $c=1856.1(4)$ pm, $\alpha=96.21(3)$, $\beta=101.49(3)$, $\gamma=93.34(3)^\circ$, $V=5900\times10^6$ pm^3, $\mu(\mathrm{Mo}_{\mathrm{K}\alpha})=5.901$ mm^{-1}, $2\Theta_{\mathrm{max.}}=50^\circ$; of 22182 reflections measured, 16085 were independent ($R_{\mathrm{int}}=0.082$) and 11914 observed with $I>2\sigma(I)$; 667 parameters (Ag, Se, P, anisotropic and C isotropic); max. residual electron density: 2.7 eÅ^3; $R_1=0.070$; $wR_2=0.18$. **2**: triclinic, space group $P\bar{1}$ (no. 2), $Z=1$, lattice constants (170 K): $a=2025.0(4)$, $b=2521.2(5)$ $c=2643.1(5)$ pm, $\alpha=61.15(2)$, $\beta=80.10(3)$, $\gamma=67.36(3)^\circ$, $V=11629\times10^6$ pm^3, $\mu(\mathrm{Mo}_{\mathrm{K}\alpha})=7.85$ mm^{-1}, $2\Theta_{\mathrm{max.}}=52^\circ$; of 64995 reflections measured, 41759 were independent ($R_{\mathrm{int}}=0.10$) and 21790 observed with $I>2\sigma(I)$; 1110 parameters (Ag, Se, P, anisotropic, C isotropic); max. residual electron density 2.8 eÅ^{-3}; $R_1=0.098$; $wR_2=0.28$. **3**: triclinic, space group $P\bar{1}$ (no. 2), $Z=1$, lattice constants (170 K): $a=2619.4(5)$, $b=2765.9(6)$ $c=2815.7(6)$ pm, $\alpha=116.39(3)$, $\beta=91.46(3)$, $\gamma=100.30(3)^\circ$, $V=17851.0\times10^6$ pm^3, $\mu(\mathrm{Mo}_{\mathrm{K}\alpha})=7.18$ mm^{-1}, $2\Theta_{\mathrm{max.}}=50^\circ$; of 56227 reflections measured, 43345 were independent ($R_{\mathrm{int}}=0.10$) and 20294 observed with $I>2\sigma(I)$; 1330 parameters (Ag, Se anisotropic, P, C isotropic); max. residual electron density 2.7 eÅ^{-3}; $R_1=0.089$; $wR_2=0.22$. **4**: triclinic, space group $P\bar{1}$ (no. 2), $Z=1$, lattice constants (170 K): $a=2824.0(6)$, $b=2980.0(6)$ $c=3225.0(6)$ pm, $\alpha=67.14(3)$, $\beta=68.02(3)$, $\gamma=67.94(3)^\circ$, $V=22333\times10^6$ pm^3, $\mu(\mathrm{Mo}_{\mathrm{K}\alpha})=9.09$ mm^{-1}, $2\Theta_{\mathrm{max.}}=48^\circ$; of 99240 reflections measured, 64156 were independent and 22753 observed with $I>2\sigma(I)$; 1933 parameters (Ag, Se, P, anisotropic, C isotropic); max. residual electron density 4.8 eÅ^{-3}; $R_1=0.12$; $wR_2=0.35$. The high R value is partly a result of the fact that a portion of the C atoms on the *n*Bu groups could not be localized. Apart from that it was not possible to distinguish the disordered solvent molecules. **5**: **5**·2THF; triclinic, space group $P\bar{1}$ (no. 2), $Z=1$, lattice constants (170 K): $a=2598.3(5)$, $b=2626.1(8)$ $c=2952.9(6)$ pm, $\alpha=112.85(3)$, $\beta=112.11(3)$, $\gamma=90.61(3)^\circ$, $V=16911\times10^6$ pm^3, $\mu(\mathrm{Mo}_{\mathrm{K}\alpha})=7.52$ mm^{-1}, $2\Theta_{\mathrm{max.}}=50^\circ$; of 70408 relections measured, 49109 were independent and 35916 observed with $I>2\sigma(I)$; 1623 parameters (Ag, Se, P, anisotropic, C isotropic); max. residual electron density 3.1 eÅ^{-3}; $R_1=0.065$; $wR_2=0.18$. Further details on the crystal structure investigation may be obtained from the Fachinformationszentrum Karlsruhe, D-76344 Eggenstein-Leopoldshafen, Germany (fax: (+49)7247-808-666; e-mail: crysdata@fiz-karlsruhe.de), on quoting the depository numbers CSD-408688 to CSD-408692.

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Detection of Catalytic Activity in Combinatorial Libraries of Heterogeneous Catalysts by IR Thermography

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The ever increasing need for more selective heterogeneous catalysts in chemical processing cannot be satisfied by conventional catalyst development and, therefore, combinatorial approaches should be considered. The combinatorial synthesis and screening of large numbers of organic compounds is already an established tool for the development of new pharmaceuticals,[1] while the combinatorial approach to the development of new solid materials has just started. In 1995 the first combinatorial developments of new materials, like new magnetoresists[2] and new superconductors[3] were reported. In 1997 libraries produced efficiently by wet-chemical syntheses with the help of ink-jet technology were created for the development of new luminescent materials.[4] New blue photoluminescent materials followed in 1998.[5] The true potential of the combinatorial approach to materials development becomes apparent by reports on thin film libraries of 25000 different materials on 7.5-cm diameter substrates. These libraries were prepared by thin film technologies using physical evaporation techniques.[6] To apply such techniques to the development of new heterogeneous catalyst materials an efficient method for the reliable spatially resolved detection of catalytic activities is required. Promising recent developments are the use of spatially resolved ionization techniques.[7] In the above-mentioned development of photoluminescent materials charge-coupled detector (CCD) cameras were applied which have excellent spatial resolution.[4–6] For the simultaneous display of catalytic activities on a catalyst library an IR-video camera appears attractive.

The applicability of IR thermography in heterogeneous catalysis was demonstrated already in 1987, where oscillations in a catalytic reaction of hydrogen with oxygen across a 4 cm^2 catalyst wafer could be monitored.[8a] Since this is a very exothermic reaction (241 kJ mol^{-1}), the temperature variations were as large as 70 °C. In the same year temperature differences smaller than 5 °C were measured for the hydrogenation of cyclohexene on Pt/SiO$_2$ catalysts with IR thermography.[8b] This technique was later applied to the screening of heterogeneous catalysts for hydrogen oxidation on 16 free-standing catalyst pellets.[9] Since the size of the catalyst pellets (4 × 3 mm) and the temperature differences observed (80 °C) limit both the spatial and the thermal resolution of these experiments, there is little prospect for application of such thermographic methods for the reliable detection of catalytic activity on large catalyst libraries with its microscopic amounts of catalysts. More promising is a recent report on the application of IR-thermographic methods for the combinatorial selection of small encoded polymer bead catalysts in

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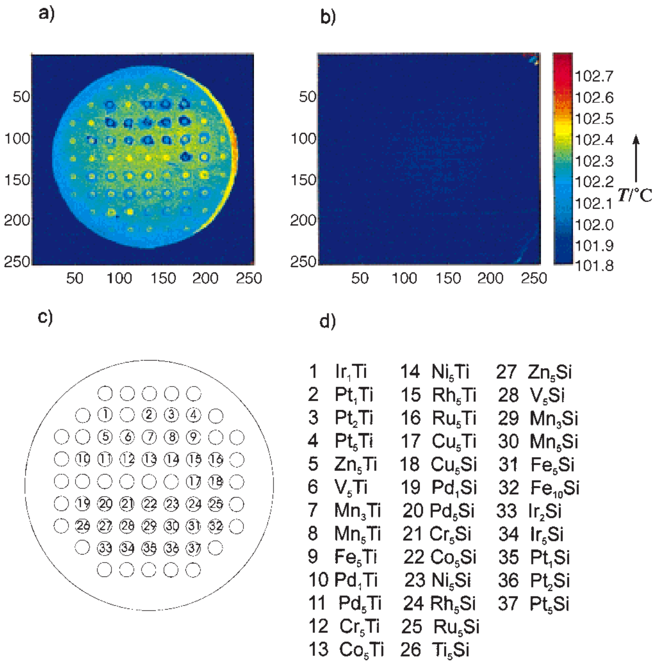
solution phase.[10] Here we report the detection of catalytic activities for heterogeneous reactions of small catalyst amounts (less than 200 µg) on a model library by IR thermography.

Visible light images mainly result from reflection and therefore require an external light source. In contrast, IR radiation is actively emitted from all objects and no external light source is required for imaging—even gases emit IR radiation. The IR image of an object is composed of emitted and reflected radiation; the relative ratio is different for each surface. The different colors on these images visualize different photon intensities of detected IR radiation. From these photon intensities blackbody temperatures can be calculated by Planck's law. These blackbody temperatures can be converted to the actual surface temperature of the object only if no reflection occurs or becomes insignificant and its emissivity is known.

Local differences in emissivity and reflectivity on a library surface and its individual catalyst spots do appear as different photon intensities, which can be misinterpreted as different temperatures, although the true surface temperatures are identical. Only at large temperature differences, like the 80 K reported,[8, 9] small differences in emissivity become negligible. When small temperature differences of a few K or smaller are to be identified, emissivity differences have to be corrected. A closely related problem is the rate of heat dissipation from tiny amounts of catalysts on the solid library. The temperature difference at the catalyst surface relative to the library surface decreases with decreasing catalyst mass. One also has to be aware that IR emission from reactants and products increases with temperature. These emissions can be reflected on the library surface causing undesired changes to the image. Therefore, IR emitters like the hydrocarbons used in our experiments can strongly affect the IR image. Our experimental design as well as our choice of IR camera were selected to reduce the effect of the above-mentioned IR-imaging problems.

Common high-sensitivity focal plane array (FPA) IR cameras are based on one of three detector materials, the semiconductors indium–antimonide (InSb), cadmium–mercury–telluride (CMT), or platinum–silicide (PtSi). InSb or CMT detector based cameras are very sensitive, but suffer from nonlinear response and a lack of long-term signal stability, which requires frequent correction and calibration of signals. The correctability and stability of the photoresponse of the PtSi-FPA detector is superior to that of the other FPA detectors.[11] We have therefore selected a PtSi-based camera, the AEGAIS from AIM equipped with a 256 × 256 PtSi-array detector and a lens with 50 mm focal length.

The primary interest of this study was to display temperature differences due to catalytic activity on a library of heterogeneous catalysts. This was achieved by applying a linear correction to the detector response and subtracting the IR image of the library just before the start of the reaction (Figure 1 a) as background (offset) from the images during an isothermal catalytic experiment. Figure 1 a shows the wells in the library surface as well as the catalyst spots due to local emissivity differences. After emissivity correction and image subtraction Figure 1 b results. The local emissivity differences of the library are no longer visible. The heat evolution due to catalytic activity can now be reliably detected since only temperature changes will be visible.



1	Ir_1Ti	14	Ni_5Ti	27	Zn_5Si
2	Pt_1Ti	15	Rh_5Ti	28	V_5Si
3	Pt_2Ti	16	Ru_5Ti	29	Mn_3Si
4	Pt_5Ti	17	Cu_5Ti	30	Mn_5Si
5	Zn_5Ti	18	Cu_5Si	31	Fe_5Si
6	V_5Ti	19	Pd_1Si	32	$Fe_{10}Si$
7	Mn_3Ti	20	Pd_5Si	33	Ir_2Si
8	Mn_5Ti	21	Cr_5Si	34	Ir_5Si
9	Fe_5Ti	22	Co_5Si	35	Pt_1Si
10	Pd_1Ti	23	Ni_5Si	36	Pt_2Si
11	Pd_5Ti	24	Rh_5Si	37	Pt_5Si
12	Cr_5Ti	25	Ru_5Si		
13	Co_5Ti	26	Ti_5Si		

Figure 1. a) IR image of the catalyst library without emissivity correction. b) Emissivity-corrected IR-thermographic image of the catalyst library prior to the start of catalytic reactions. The bar on the right gives the temperature/color key of the temperature window [°C]. c) Deposition pattern of the library. d) Composition of the oxide catalyst spots of the library according to the AMM notation (the molar percentages of active metal and base metal oxide are given, that is AMM-Ti_3Si stands for 3 mol% titania in 97 mol% silica).

To avoid reflections at the catalyst library, a slate plate of low reflectivity was chosen as substrate. The effects of thermal IR emission from hydrocarbon reactants and products in the gas phase were reduced by the use of a 3.6-µm cut-on IR filter.

Owing to the rapid development of combinatorial chemistry the principal preparation of large libraries by evaporation techniques[2, 3, 5, 6] or wet-chemical deposition [4] even at higher pressures[12] is already state of the art. Our model library of new catalyst materials was based on the sol–gel procedure for the preparation of amorphous microporous mixed oxides (AMM). AMM materials show a monomodal narrow micropore size distribution, a large surface area, high porosity, and a homogeneous dispersion of the catalytically active centers in the materials (no domains). Thus a large variety of catalytically active elements can be atomically dispersed in the shape-selective environment of micropores. These materials have already shown unusual properties as powder catalysts or as catalytic membranes in selective oxidations, hydrocracking, hydrogenations, etherifications, and esterifications.[13] The vast number of AMM materials preparable makes this class of materials a promising target for combinatorial searches of catalytic activities. The individual sols identified in Figure 1 d were deposited in amounts of 1.5–5 µL corresponding to less than 200 µg of final catalyst spots in the small wells on the surface of the slate substrate, followed by controlled drying, and calcination of the library. Figure 1 c and 1 d show the library and its chemical composition. The

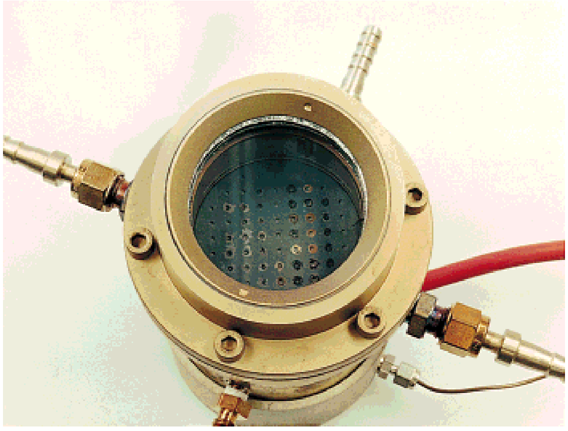


Figure 2. Photograph of the reactor with a mounted library.

reactor has been equipped with a large IR-transparent BaF_2 window (Figure 2). The calcined library was placed in the reactor and reduced at 300 °C for 3 h under a constant flow of hydrogen prior to the experiments. As test reactions the hydrogenation of 1-hexyne at 100 °C and the oxidation of isooctane and toluene at 350 °C were chosen.

Figure 3 shows the corrected IR image of the library surface during the hydrogenation of 1-hexyne at 100 °C. Of the 37 catalysts only four appear catalytically active, that is the AMM-Pd_1Si, and AMM-Pd_5Si on the left as well as AMM-Pt_2Si and AMM-Pt_5Si on the right. The clean image obtained is remarkable, since it results from 2–20 µg Pd or Pt in the AMM matrix. Temperature differences of 0.1 K are clearly resolved, while the highest temperature difference obtained does not exceed 0.7 °C.

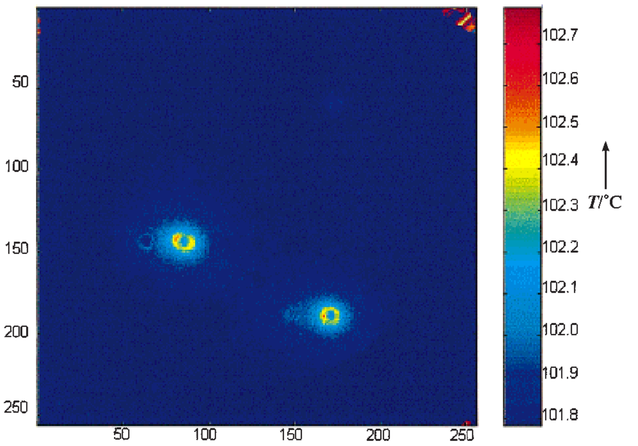


Figure 3. Emissivity corrected IR-thermographic image of the catalyst library during 1-hexyne hydrogenation in the gas phase at 100 °C. According to IR-thermographic measurements the temperature of the library was 101.8 °C.

On the same library by increasing the temperature to 350 °C and switching the gas-phase flow to Ar and then to air and isooctane, catalytic oxidation properties were examined. Figure 4a shows the results. Now the AMM-Ti materials were more active than the AMM-Si based catalysts. For the catalytic isooctane oxidation (Figure 4a) the catalyst samples AMM-Pt_1Ti, -Pt_2Ti, -V_5Ti, -Pd_1Ti, -Ru_5Ti, and -Cu_5Ti show activity. Since aromatic compounds usually show a different behavior towards catalytic oxidation, the oxidation of toluene was examined (Figure 4b). The difference observed relative to the isooctane oxidation was larger than expected. Figure 4b shows that AMM-Pd_1Ti, which was very active in isooctane oxidation, is now inactive, while the AMM-Pt_5Si, inactive in the oxidation of isooctane, is now one of the most active materials. AMM-Pt_5Ti, while active in the toluene oxidation, shows low activity for isooctane oxidation. Like in the isooctane oxidation AMM-Pt_1Ti, -Pt_2Ti, -V_5Ti, and -Cu_5Ti are active catalysts. For both oxidation experiments the actual temperature difference detected by the camera was 1 to 2 °C. This is significantly larger than the temperature difference in the hydrogenation reaction, which reflects the higher exothermicity of these reactions.

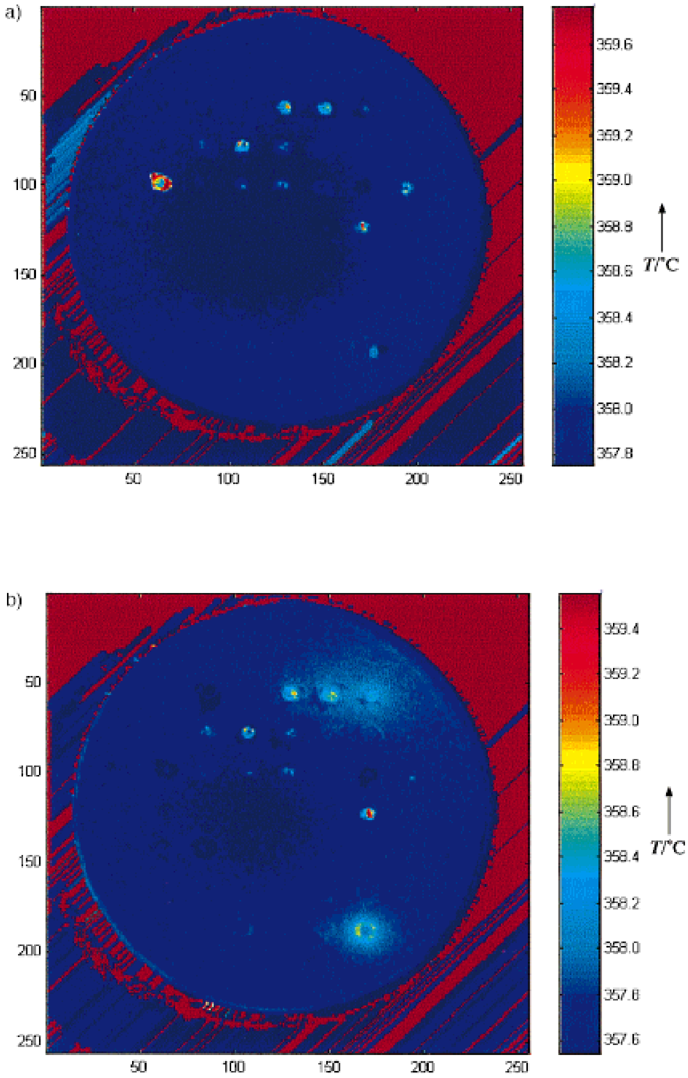


Figure 4. Emissivity-corrected IR-thermographic images of the catalyst library during isooctane oxidation in the gas phase at 350 °C (a) and of the catalyst library during toluene oxidation in the gas phase at 350 °C (b). According to IR-thermographic measurements the temperature of the library was 357.7 °C.

We have demonstrated that, after careful removal of artefacts, IR imaging is a very powerful tool for the detection of catalytic activities on combinatorial libraries. Temperature differences down to 0.1 K can reliably be detected and the heat evolution of catalyzed gas-phase reactions on small catalyst amounts (< 200 μg) identified. Reactions have been observed at temperatures up to 350 °C, indicating that the method can be applied over a wide temperature range. The method has also been applied successfully to the detection and screening of enantioselectivity in liquid-phase reactions (see the following communication),[14] stressing its general usefulness.

Clearly, high-throughput screening of larger libraries could now be achieved with IR imaging of catalyst activity. We are presently engaged in the adjustment of a robotic system for automated library preparation, automated quantification of the heat response of the individual samples on the library with the help of software, and improvement of the signal sensitivity of the camera setup. Detection of catalytic activity in combinatorial libraries reduces the time necessary to find new potential catalysts. The development of the most promising candidates into useful new catalyst materials still requires more conventional laboratory techniques.

Experimental Section

For the sol preparations tetraethoxysilane (TEOS) was used as the silica precursor and tetraisopropoxytitanium as titania percursor. The following precursors were used for the other elements: $PdCl_2$, Na_2PtCl_6, $IrCl_4 \cdot xH_2O$, $RuCl_3 \cdot xH_2O$, $CoCl_2 \cdot 6H_2O$, $[Fe(acac)_3]$, $[Mn(acac)_3]$, $(iPrO)_3VO$, $CrCl_3 \cdot 6H_2O$, $[Cu(acac)_2]$, $[Ni(acac)_2]$, $ZnCl_2$, $[Pd(acac)_2]$.

Preparation of sols: The silica sols were prepared according to the standard procedure by Klein et al.[12] The compounds were used in the molar ratios for the sol preparation as indicated by the AMM notation.

The titania sols were prepared by dissolving titanium isopropoxide (3.36 mmol, 1 mL) in dry ethanol (3.33 mL) while stirring. After the mixture had been stirred for 30 min, 8 N HCl (8.33 μL) was added. After 5 min, concentrated HCl (46.7 μmol) was slowly added over about 20 min, then ethanol (833 μL), and finally an ethanolic solution (833 μL) of the metal precursor.

Preparation of the catalyst library: The catalyst library was prepared by pipetting μL amounts of titania or silica sols into the wells (diameter 1.5 mm, depth 0.6 mm) of the slate library substrate. In the case of the silica sols 1.5 μL (equivalent to 192 μg silica catalyst) and in the case of the titania sols 5 μL (equivalent to 182 μg of titania catalyst) were deposited. After evaporation of the solvent the library was heated to 65 °C with a heating rate of 1 °C min^{-1} and kept at that temperature for 30 min. Then the temperature was increased to 250 °C (heating rate of 1 °C min^{-1}) where it was kept for 180 min. The library was then allowed to cool down to room temperature at a rate of about 1 °C min^{-1}.

Correction and calibration procedure of the IR-camera system: The detector response was corrected prior to the catalytic reaction by a two-point correction taking images of the library at temperatures 5 °C above and below the desired reaction temperature (hydrogenation: 100 °C, oxidation: 350 °C). Before the organic reactant was evaporated into the feed flow of hydrogen or synthetic air, an IR image of the library was taken and subtracted as background. To assign a temperature scale to the IR images six calibration measurements were performed for each experiment taking images of the library at six different temperatures. By fitting a quadratic polynome to the pixels of the calibration images temperature values were assigned to the different colors of all corrected images.

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Time-Resolved IR-Thermographic Detection and Screening of Enantioselectivity in Catalytic Reactions

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Klaus M. Kühling, and Arnold Holzwarth

*Dedicated to Professor Gernot Boche
on the occasion of his 60th birthday*

The development of chiral homogeneous metal catalysts and biocatalysts for the enantioselective synthesis of optically active compounds is of considerable academic and industrial interest.[1] Traditionally such catalysts have been prepared and studied one by one, which is extremely time-consuming. Following the advent of combinatorial methods in pharmaceutical research,[2] a few attempts have been made to apply certain aspects of combinatorial chemistry to asymmetric catalysis.[3] So far success has been limited, one reason being the lack of efficient methods for rapid screening of enantioselective reactions. Recently we showed how in-vitro evolu-

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